OAK RIDGE NATIONAL LABORATORY
Transportation Program

Fiscal Year 2005 Transportation Program Highlights

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Introduction

The Oak Ridge National Laboratory (ORNL) Transportation Program supports the mission of the FreedomCAR and Vehicle Technologies (FCVT) Program, a part of the Department of Energy's (DOE's), Office of Energy Efficiency and Renewable Energy (EERE). The Program aims to develop more energy-efficient and environmentally friendly highway transportation technologies that enable America to reduce petroleum usage. ORNL conducts pre-competitive research and development (R&D) on a wide range of technologies, including 1) advanced combustion regimes in vehicle engines; 2) the effects of fuel properties on engine efficiency and emissions; 3) power electronics and electric machines; and 4) advanced materials that are strong, lightweight, and durable.

The Program supplements in-house expertise and facilities through subcontracts with private industry and universities to provide specialized analysis, equipment, technical services, and so forth. In addition, partnerships with industry are an important part of developing transportation technologies. Partnerships are executed through a variety of mechanisms, including Cooperative Research and Development Agreements (CRADAs), user agreements, and cost-shared subcontracts. These partnerships ensure that ORNL's R&D activities address the technical barriers faced by industry, such as creating advanced technology components and vehicles that offer increased fuel efficiency and meet 2007 and 2010 Environmental Protection Agency (EPA) emission standards. The Transportation Program also addresses the longer-term national goals of decreasing and eventually eliminating dependency on imported oil in the transportation sector. ORNL R&D activities in power electronics and energy storage are applicable to hybrid and plug-in electric vehicles in the short term and fuel cell-powered automobiles in the long term. Projects to develop clean, efficient diesel engines and diesel exhaust aftertreatment systems enable the use of fuel-efficient diesel engines in light-duty vehicles. Such projects also contribute to 21st Century Truck Partnership (21st CTP) goals to increase efficiency, reduce emissions, and improve safety and economy in medium and heavy-duty trucks. Materials R&D projects support and enable the development of these innovative technologies for both light-duty and heavy-duty vehicle applications.

ORNL's Transportation Program received approximately $41.5 million in new budget authority in fiscal year (FY) 2005. The Program expended $11 million in R&D subcontracts, much of which was supplemented by substantive cost sharing. The Program supported approximately 190 full time-equivalent ORNL scientific and technical staff, and two national user facilities: the National Transportation Research Center (NTRC) and the High Temperature Materials Laboratory (HTML). This research resulted in over 300 presentations and publications, and 20 patent disclosures. During FY 2005, 11 patents were awarded as a result of earlier disclosures.

In FY 2005, Edmund T. Grostick served as the ORNL Transportation Program's Acting Program Director. During Mr. Grostick's time with the Program, the ORNL Transportation Program attained its first "outstanding" performance rating from DOE. In July 2005, Mr. Grostick retired from this position and was succeeded by Dr. Raymond G. Boeman as Transportation Program

Director. Dr. Boeman received his PhD in Engineering Mechanics from Virginia Polytechnic Institute and State University in 1990. Since joining ORNL in January 1991, Dr. Boeman has played a vital role in transportation research. After successfully managing an automotive adhesives research project at ORNL, Dr. Boeman took a one-year assignment in Detroit, MI, to work with the Automotive Composites Consortium. This one-year assignment turned into five years of working hand-in-hand with U.S. automakers. In the spring of 2004, Dr. Boeman accepted a new assignment with DOE in Washington, DC, providing technical assistance to the 21st CTP through the FCVT Program. After the completion of this assignment, Dr. Boeman has returned to ORNL and taken over management of the Transportation Program. His experience with industry and DOE will be a tremendous asset for the Program.

This report is organized in two sections: 1) Project Summaries and 2) Technical Highlights. The Project Summaries section provides brief overviews of the Transportation Program's activities in FY 2005. The Technical Highlights section includes detailed descriptions of noteworthy research results and technical achievements.

Project Summaries

National Transportation Research Center

In the last quarter of FY 2005, NTRC emphasized establishing a user base to increase the number of user agreements for the Test Machine for Automotive Crashworthiness (TMAC). A TMAC information package was assembled, potential TMAC users were contacted, and a targeted development effort was mounted within the ACC Energy Management group. Proposals from user candidates are expected in FY 2006 as a result.

In FY 2005, three organizations inquired about establishing user agreements with NTRC, but none resulted in a signed user agreement. A heavy vehicle dynamics and rollover project was completed, bringing ORNL together with Dana, Michelin, and National Transportation Research Center, Inc. (NTRCI). The project studied vehicle rollover characteristics of a conventional tractor/box trailer configuration, first using dual tires and then substituting next-generation single tires. Results showed a stability improvement with the next-generation single tires. A paper was submitted to the International Truck and Bus Safety and Security Symposium and was subsequently selected as one of four outstanding symposium papers. This successful industry-laboratory relationship contributed to the formation of an outstanding team that included ORNL and Dana in an FCVT-funded FY 2005 heavy-duty cycle project. The project will extend through FY 2006 and involves instrumenting a heavy-duty tractor and trailer combination. The instrumentation will collect data on characteristics such as fuel usage, engine operating parameters, emissions stability, and other details (e.g., weather conditions) related to the long-haul driving environment. The data will be used in computer models that can be used by engineers, designers and manufacturers to develop heavy-duty vehicles that are lighter, safer, more fuel-efficient, and friendlier to the environment.

Planning and negotiation continued for the development of a new facility co-located with NTRC. This facility, which will be called the Energy Conversion Research Facility (ECRF), would primarily provide additional analytical and engine test cell space for the Fuels, Engines, and Emissions Research Center (FEERC); facilities for alternative liquid and gaseous fuels R&D; facilities for distributed energy power plant R&D; and bench-scale analytic and experimental facilities for fuel cell R&D. The envisioned facility will be about 31,000 square feet. Just over half will be dedicated to research space and the remaining to research support. Similar to NTRC, ECRF is expected to be built by or leased from a private third party. The facility could be ready for occupancy as early as FY 2007.

The ORNL Business Management Division has calculated the FY 2005 cost savings derived from housing researchers at NTRC rather than on the main ORNL campus to be approximately $987,000, for a cumulative savings (FY 2002-2005) of approximately $3,783,400.

High Temperature Materials Laboratory

In FY 2005, the High Temperature Materials Laboratory (HTML) User Program received a record high of 110 user proposals. Of these, 21 were from first-time user institutions, and the number of user agreements with ORNL increased from previous years with 33 new agreements signed (27 from industrial concerns and six from colleges and universities).

The sub-angstrom resolution electron microscope [Aberration Corrected Electron Microscope (ACEM)] became functional in FY 2005. With the ability to exhibit single-atom resolution, the ACEM was used on several FCVT-sponsored projects on prototypical catalyst materials (i.e., atoms atomically-dispersed on an alumina substrate). Other HTML user projects and FCVT-sponsored projects have been accepted for future work using the ACEM.

Improvements to the Neutron Residual Stress Facility (NRSF-2) were completed in FY 2005, and related user projects were initiated. As one of the first users of the facility, Caterpillar investigated a new welding procedure. The procedure promised to be more rapid and less costly than the current one in use, but Caterpillar needed to know if it produced the same or less residual stress. Caterpillar used the NRSF-2 facilities to measure the residual stress. The new NRSF-2 has a higher number of detectors, a faster response time, a higher neutron flux on the sample, more robust specimen holders (capable of supporting hundreds of kilograms), and more flexibility. The facility also houses a furnace, mechanical testing stage, and atmospheric control capability. These improvements to NRSF-2 have made it a unique, world-class facility.

With the Spallation Neutron Source (SNS) nearing completion, HTML moved forward in its plans for the VULCAN "engineering materials diffractometer" (located at SNS). In FY 2005, HTML was able to 1) provide staff support to the SNS-VULCAN instrument development team, 2) design and build an off-spectrometer specimen alignment system, and 3) procure additional detectors.

Of the 110 proposals received in FY 2005, 38 were on subjects directly relevant to FCVT. These included projects in areas such as aluminum and aluminum matrix composites, magnesium and its composites, high-strength steels, diesel particulate filters, exhaust emission catalysts, and both hydrogen-internal combustion engine (ICE) and diesel engine fuel injector components. Thirteen projects were not directly relevant to FCVT but did involve transportation-related projects such as welding and weld structural quality examination, metal casting, spark plug development, new high-strength bulk metallic glasses, and thermal properties of engine coolant additives. Other projects (39) were relevant to other EERE topics like hydrogen storage, hydrogen membranes, fuel cells, and even solar cell materials. In addition, 34 projects were relevant to other areas, including high-speed or high-power electronic materials and components, titanium alloys for medical implants, catalysts for bioprocessing, and numerous basic research projects on nanomaterials.

Advanced Power Electronics

ORNL's Power Electronics and Electric Machinery Research Center (PEEMRC) at NTRC conducts high-risk, long-term research, evaluates hardware, and provides technical support to the FCVT Program's Advanced Power Electronics and Electric Machines (APEEM) activity. Through PEEMRC, ORNL serves on the FreedomCAR Electrical and Electronics Technical Team. ORNL researchers evaluate technical proposals for DOE and lend their technological expertise to the evaluation of projects and developing technologies. ORNL executes specific projects for DOE in power electronics, electric machines, and thermal control, in order to help remove technical and cost barriers so that technologies will be suitable for use in advanced vehicles that meet the goals of FCVT. This provides a portfolio of options that automotive manufacturers and suppliers can use when developing their unique solutions for hybrid and fuel cell vehicles.

Significant progress was made in FY 2005 in the development of advanced electric machines and power electronics components for hybrid electric vehicles (HEVs) and fuel cell–powered vehicles. A prototype radial gap interior permanent magnet motor with external field excitation was built. Test results showed a doubling of the torque at the same full-load current. Additionally, it can increase the motor's speed range and provide both field weakening and enhancement. Testing of the prototype successfully demonstrated the field weakening and enhancement features of this concept.

An integrated DC-DC converter topology was also built and tested by ORNL. The technology employs only four switches while providing a triple voltage bus (14 V/42 V/high voltage). The integrated converter should provide greater reliability, reduced cost, and reduced size, while providing the multiple voltages required by HEVs and fuel cell vehicles. Further cost savings are realized by eliminating the inductor. Simulation studies verified the functionality of the topology and indicated an operating efficiency of 93 percent between 30 and 70 percent of full load. A 2-kW prototype was fabricated and functional testing proved the concept.

ORNL developed an integrated traction and compressor drive system which shares components for the two functions. For the compressor drive, the number of inverter components, including semiconductor switches and gate drive circuits, were reduced by more than one-third. The compressor drive control was incorporated into the traction motor controller, rather than having a separate control circuit, further reducing the cost. ORNL tested a prototype inverter with a three-phase induction motor and a two-phase compressor motor. These tests demonstrated that the inverter concept can drive either motor separately or both motors simultaneously without affecting the other's operation.

Additionally in FY 2005, a novel thermal control system was developed by ORNL. This concept uses refrigerant from the vehicle air conditioning system to provide thermal control for an inverter and motor specifically designed to use this coolant. Because this coolant system integrates with the high-temperature side of the vehicle's air conditioning (A/C) system, it does not use the compressor and results in a coefficient of performance (COP) of 30 or greater. A prototype system was designed and fabricated using an automotive A/C system. System integration issues associated with refrigerant migration and system dynamic performance were resolved and design activities were initiated for the motor and inverter. Heat transfer studies demonstrated a heat flux in excess of 150 W/cm^2. By efficiently cooling the inverter and motor, it will be possible to reduce the size of the inverter by two-thirds.

Fuels, Engines, and Emissions

ORNL's Fuels, Engines, and Emissions Research Center (FEERC), located at NTRC, conducted R&D for multiple subprograms of the FCVT Program in FY 2005, including Advanced Combustion and Engine R&D, Fuels Technology, and Vehicle Systems. Through FEERC, ORNL has collaborated with industry through five CRADAs in engine/emissions technology, as well as through less-formal, but very active collaborations with approximately 15 additional private companies and non-DOE agencies. Several of the CRADAs have resulted in the installation of unique research hardware at FEERC. In addition, six private sector firms sponsored R&D at the center in FY 2005. FEERC held its third Guidance and Evaluation Panel meeting in November 2004, with members from Ford, Cummins, BP-Amoco, Caterpillar, Umicore, and others.

Researchers at FEERC are highly engaged in supporting FreedomCAR and Fuel Partnership and 21st CTP programmatic activities, including the Advanced Combustion and Emission Control Technical Team, the Diesel Crosscut Team, and the 21st CTP Lab Council. ORNL provides co-leadership with industry through the Crosscut Lean Exhaust Emissions Reduction Simulation (CLEERS) activity. In fuels technology, FEERC staff members co-chair three subteams of the Advanced Petroleum Based Fuels-Diesel Emission Control project and sit on the steering committee in partnership with the National Renewable Energy Laboratory (NREL). Researchers at FEERC also participate in working groups for the Coordinating Research Council. FEERC staff and facilities play significant roles in the Advanced Reciprocating Engine Systems (ARES) projects in the Distributed Energy Program. Both FCVT and ARES benefit from this leveraging.

In FY 2005, there were a number of additions to capabilities at FEERC in order to stay current with the challenges and research requirements of the Center's partners and DOE. These include:

- A variable compression ratio engine was developed for ORNL;
- A unique, camless diesel research engine from CRADA partner International Truck and Engine Corporation; and
- Hydrogen fuel capability was added for engine and nitrogen oxides (NO_x) aftertreatment studies.

Advanced combustion engines research is undergoing an orderly shift to more emphasis on improving engine fuel economy through advanced combustion regimes and other technologies, while retaining critical projects on key remaining issues in emission controls.

ORNL participates with 14 other organizations in a Memorandum of Understanding (MOU) on Advanced Engine Combustion Research. ORNL's specific roles in the MOU are: 1) determining how advanced combustion regimes might be exploited for inherent efficiency gains; 2) determining the detailed emissions species generated by these combustion regimes; and 3) researching control strategies for full power density and transitions. Powerful capabilities in engine electronic control prototyping were exercised to show quick and near-seamless transitions between operating points within the low-temperature combustion (LTC) operating environment.

Although most LTC emphasis has been based on diesel fuel, gasoline-based homogeneous charge compression ignition (HCCI) engines can potentially yield higher efficiency than conventional spark-ignition engines and can also reduce emissions. ORNL has been studying the use of spark augmentation for stabilizing the cycle-to-cycle efficiency variation encountered in certain types of mixed-mode (conventional and HCCI) engines. Researchers have found that the cyclic dispersion encountered during the conventional-to-HCCI operation transition is complex (high period or deterministic chaos with noise) but is short-time predictable. This indicates that it may be possible to develop proactive control algorithms for stabilizing HCCI and for these transitions, helping expand the overall operating range.

Research on improving the efficiency of lean nitrogen oxide (NO_x) trap (LNT) regeneration led to a new strategy that integrated the features (low NO_x and high hydrocarbon)] of LTC with mild fuel enrichment to de-NO_x the LNT. The technique provides five to ten times the NO_x reduction per unit of excess fuel.

An engine management strategy was identified that can produce moderate levels of hydrogen in the engine exhaust in overall lean operation that would enhance the performance of lean-NO_x catalysts. The experiments to confirm this were requested by an automobile OEM.

The CLEERS team continued development and validation of a standard protocol for LNTs. The success of the LNT collaboration has provided a framework for similar data sharing and collaborations among CLEERS team members for urea-SCR (selective catalytic reduction) and diesel particle filter technologies. The team also maintained the website (http://www.cleers.org) and organized the eighth CLEERS workshop.

An extensive study of fuel property effects on both gasoline-based and diesel-based HCCI performance and emissions was completed. Results were published showing that the fuel properties could in fact expand or shrink the HCCI operating space in the case of gasoline fuels. For diesel-like fuels, the results show how the cool-flame reactions are prominent in fuels with a high cetane number. To more globally facilitate and coordinate research in this area, ORNL conceived a vision to initiate a comprehensive project on how fuel properties affect advanced combustion processes like HCCI. ORNL teamed with NREL to move the project plans forward. The effort will begin with design of a research fuel matrix via a working group of experts in this field convened under the auspices of the Coordinating Research Council. This project has been named FACE (fuels for advanced combustion engines).

ORNL supports the FCVT Vehicle Systems Team in cost modeling for advanced vehicle components, and in developing performance/emissions models for engine and exhaust aftertreatment components. In FY 2005, the efforts were redirected to aid the development of the Powertrain Systems Analysis Toolkit (PSAT) code in conjunction with Argonne National Laboratory (ANL). Johney Green, FEERC group leader, has been appointed to the FreedomCAR Systems Technical Team and is serving as a liaison to the Advanced Combustion and Emission Control Technical Team.

FEERC also contributed to FCVT's Environmental Impacts and Health Impacts activities in FY 2005 by assisting in the determination of the potential adverse impacts of new FCVT technologies being developed. The Watt Road Environmental Laboratory received FY 2005 funding from the FCVT Health Impacts activity for real-world truck emissions studies. Department of Transportation (DOT) and EPA have co-sponsored certain studies at the Watt Road laboratory. Ambient sampling of particulate matter and formaldehyde near the truck stop that is included in the field laboratory site has shown a strong variation throughout the day and dependence on ambient conditions. In-cab emissions sampling has been provided to show the impact of nearby idling trucks versus the in-cab levels just from idling the subject truck.

For FY 2006 and beyond, FEERC expects to continue activities in the combustion MOU with increased emphasis on engine efficiency improvements. In fuel technologies, matching fuel properties to advanced combustion will be addressed in the FACE project. In parallel, the critical remaining issues in emission controls must be addressed. CLEERS is expected to remain a focal point of those efforts.

Automotive Lightweighting Materials

ORNL supports the FCVT Program's Automotive Lightweighting Materials (ALM) activity by focusing on structural materials for vehicle body and chassis applications. ORNL looks specifically at those materials which have the potential to significantly reduce the weight of passenger vehicles without compromising vehicle lifecycle cost, performance, safety or recyclability. ALM's goals include developing and validating advanced material technologies by 2012 that, if implemented in high volume, could cost-effectively reduce the weight of body and chassis components by at least 60 percent with performance, reliability and safety characteristics comparable to those of conventional vehicle materials. ORNL conducts R&D activities in ALM research areas such as cost reduction, design data and modeling, manufacturability, tooling and prototyping, joining and assembly, performance enhancement, and maintenance. Efforts are further organized into activities in automotive metals, polymer composites, low cost carbon fiber, materials joining, non-destructive evaluation, and enabling technologies.

In FY 2005, ORNL demonstrated substantial progress in carbon fiber reinforced polymer matrix composites. Because of their high stiffness and strength, these composites offer to potentially reduce vehicle weight by more than 50 percent. The current barrier, however, to implementing these in automotive systems, is the cost of carbon fiber. During the past few years, the Program has been developing technologies aimed at reducing the cost of carbon fiber by focusing on both the raw materials and the processing methods being used. The Program is developing methods to rapidly and inexpensively stabilize, oxidize, carbonize, graphitize, and post-treat commercial grade carbon fibers, as well as using lower-cost starting materials.

In order to commercialize these technologies, they must first be merged into a single processing line that allows the application of a user-selected number of the new technologies with conventional processing technologies. The integration line, which is currently under development, will allow manufacturers to pick and choose which of the new technologies they wish to employ and resolve interface issues between conventional and advanced technologies prior to the design of new commercial lines. The program has established and brought the conventional part of the processing line to full operation and has designed and built the first full-scale unit of the advanced technology line.

Additionally in FY 2005, ORNL developed new experiments for the characterization of progressive crush of Advanced High Strength Steels (AHSS). New developments in AHSS metallurgy and processing, combined with computer and modeling advancements, require accurate material characterization and verified models in order to fully utilize the increased strengths of the materials. The TMAC was used to provide high quality component level data for development of material and structural computer models. Validated models were distributed to steel manufacturers and automotive designers and enable more accurate modeling and design of lightweight crashworthy vehicles.

High Strength Weight Reduction Materials

The FCVT Program's High Strength Weight Reduction (HSWR) Materials activity focuses on cost-effectively reducing parasitic energy losses due to the weight of heavy vehicles, without reducing vehicle functionality, durability, reliability, or safety. ORNL contributes to the goals of the HSWR activity, which are primarily aimed at applications in Class 8 trucks. These trucks consume more fuel annually than Classes 3 through 7 combined. HSWR activity goals support those of the 21st CTP to reduce the weight of an unloaded tractor-trailer combination from the current 23,000 lb to 18,000 lb by 2012. These goals are to be met so that performance, durability, reliability, and safety characteristics, as well as cost-competitiveness, are comparable to those of conventional vehicle materials. The HSWR activity is pursuing research in numerous technical areas, including cost reduction, design data and modeling, manufacturability, tooling and prototyping, joining and assembly, performance enhancement, and maintenance, repair and recycling. The use of lightweight materials in heavy vehicles presents significant technical challenges to the existing body-assembly joining processes such as resistance spot welding.

At ORNL, researchers are working on the ultrasonic welding process. This is a solid-state joining process and addresses the critical industry need for increased use of lightweight and high-performance materials in heavy-duty vehicles. Initial focus has been on identifying potential applications with industry partners, developing application-specific demonstrations, and fostering technology partnerships. Presently, aluminum, steel and magnesium have been successfully ultrasonically welded. This technique is extremely energy efficient, due to the nature of the solid-state process, and it offers high productivity due to its fast cycle time.

Also in FY 2005, researchers from ORNL and Pacific Northwest National Laboratory (PNNL) began evaluating and designing composite-composite and composite-metal joints. Even when lower-cost carbon fiber becomes available and component processing methods are fully developed, major system design issues will remain where composite materials are joined to other composites and to other metallic materials. In this effort, researchers are developing technically robust and economically attractive joining techniques for attaching a variety of light and heavy materials. Researchers have worked closely with AlphaSTAR to develop and validate an interface between GENOA and the ABAQUS solver, which allows for contact modeling. This is critical for investigating damage in the composite at a bolted joint.

In addition, in FY 2005, a new ASTM standard practice for friction testing was approved and became available for diesel engine designers and manufacturers.

Automotive Propulsion Materials

The FCVT Program's Automotive Propulsion Materials (APM) activity focuses on developing materials technologies that are critical to the 1) advanced power electronics and 2) compression-ignition direct-injection (CIDI) engine and emissions control research areas. The activity supports these two core technology areas by providing materials expertise, testing capabilities, and technical solutions for materials problems. The activity provides component development, materials processing, and characterization to enable successful development of efficient electric drive systems and emissions-compliant CIDI engines.

APM projects at ORNL address materials concerns that directly impact the critical technical barriers in each of the activity's core technology areas mentioned above. These barriers involve fundamental, high-risk materials issues, such as thermal management, emissions reduction, and reduced manufacturing costs.

In FY 2005, a test facility was developed at ORNL to aid designers of automotive components that use permanent magnets to determine how the properties of magnets change as a function of temperature and thermal cycling.

Heavy Vehicle Propulsion Materials

Advanced materials are an enabling technology for fuel-efficient, heavy-vehicle truck engines. Major progress was made in the development of heavy vehicle propulsion materials in FY 2005 including materials for exhaust aftertreatment and materials for air handling, hot section, and structural applications.

The reduction of NO_x and particulate emissions is critically important to the FCVT Program and is highly materials dependent. DOE goals for improved efficiency of heavy vehicles are greatly complicated by engine design and exhaust aftertreatment technologies designed to meet the mandatory EPA emission regulations for 2007 and 2010. Materials and systems research is being conducted to minimize the potentially negative effects of emission-reduction technologies on fuel economy and to result in cleaner and more efficient engines.

ORNL is conducting an integrated effort in diesel engine exhaust aftertreatment, using unique expertise and facilities in ultra-high resolution scanning transmission electron microscopy and high performance computational Density Functional Theory modeling of catalyst behavior to determine the atomic mechanisms of catalyst coarsening and loss of effectiveness in diesel exhaust environments. ORNL is also collaborating with a major diesel engine manufacturer to develop materials analysis tools (X-ray diffraction, Raman spectroscopy, and electron microscopy) for studying catalyst behavior in all stages of the life of the catalyst and determining the parameters that control the life of the aftertreatment device. The lessons learned from these theoretical and experimental observations of catalyst behavior are used as a guide to the development and testing of improved catalyst systems.

ORNL is also collaborating with a diesel engine manufacturer and a domestic supplier of diesel particulate filters to develop an understanding and quantitative model of the durability and expected lifetime of diesel particulate filters. The results of this effort will contribute to the improvement of the filter, development of nondestructive inspection techniques for use during routine engine servicing, and predictions of filter lifetime to facilitate timely replacement.

In a collaborative effort with a domestic automotive company and Lawrence Livermore National Laboratory (LLNL), ORNL is developing an on-vehicle NO_x sensor to enable anticipated exhaust aftertreatment technologies such as the lean NO_x trap and selective catalytic reduction.

Frictional losses in commercial diesel engines represent a significant loss of fuel efficiency. ORNL is developing surface modification technologies to reduce frictional losses in engine components. For example, a simple, low-cost process was developed to greatly improve the frictional behavior of titanium components.

The useful life of engine components can be modeled and predicted via life-prediction testing and modeling methodology developed over the past 20 years by DOE, NASA, and other contributors. ORNL has extended the state-of-the-art life prediction methodology to the microscopic level via the development of copyrighted microstructure-based finite element analysis (FEA) software. The "micro FEA" program uses microstructural images from component materials and commercial FEA codes to predict stresses in components at the microscopic level.

Vehicle Systems

The FCVT Vehicle Systems subprogram at ORNL is principally constituted by simulation and validation projects conducted in conjunction with other national laboratories and industrial partners. ORNL plans to strengthen and increase collaborations with other national laboratories (chiefly ANL) and pursue niche activities that add value to FCVT's systems analysis portfolio.

In FY 2005, ORNL made significant progress in establishing life cycle cost estimation as part of the Powertrain Systems Analysis Toolkit (PSAT), DOE's preferred platform for vehicle systems analytical work. Specific technical accomplishments in this task were highlighted by considerable integration of PSAT and ORNL's Advanced System Cost Model (ASCM). ASCM estimates generic production cost of advanced vehicle configurations, and supplements detailed models at the vehicle subsystem level. Thirteen different light-duty vehicle size classes were studied in FY 2005, with several different powertrain options (including series hybrid, parallel hybrid, fuel cell, etc.). Additionally, a joint ORNL/ANL paper on the cost modeling effort was presented in an international forum (EVS-21) in May 2005. Emphasis in FY 2006 will be on construction of a heavy truck model in partnership with other national laboratories.

Although late in the fiscal year, ORNL re-energized its aftertreatment device modeling effort. This activity has already picked up momentum in the first quarter of FY 2006 and will expand to include advanced combustion modes (e.g., low temperature combustion) and engine configurations (e.g., cylinder deactivation). Researchers at ORNL believe there is exceptionally useful information in the data gathered under the CLEERS project (under the Diesel Crosscut Team) that is not being fully utilized. Early guidance in establishing CLEERS stipulated that the effort was not to produce models, but rather the empirical data from which industry partners and others could build their own models. ORNL and other CLEERS partners have established some "proto-models" which are mathematical expressions of observed behavior (emissions chemistry, etc.). These proto-models have promoted macro-device modeling, and ORNL is proposing further extension of aftertreatment modeling using CLEERS data.

The Heavy Vehicle Drive Cycle project had a new start in FY 2005 and made good progress in initiating the identification of desired information and the necessary on-board sensors, instruments, and data acquisition systems. Significant industry cooperation in commencing on-road cycle runs was obtained as well.

Energy Storage

The Condensed Matter Science Division and the Metals and Ceramics Division of ORNL are collaborating to develop new materials to address some of the key challenges for advanced battery technology. Great progress has been made to improve the lithium-ion battery technology in recent years, but the need for batteries with higher specific energy and power densities, lower cost, safe and robust performance over a 10-year lifetime is particularly acute for the hybrid electric vehicle and full electric vehicle activities.

In FY 2005, research focused on two designs for advanced cathodes for lithium batteries. One of these designs was based on using graphite foam as the support and current collector. The graphite foams developed at ORNL have remarkably high electronic and thermal conductivities that may help alleviate the safety concerns of thermal runaway in lithium-ion batteries. The pore size, density, surface area, and graphitization of the foams can be widely tailored to optimize the electrode performance. Promising results were obtained by coating graphite foam plates with an active battery material, $LiFePO_4$. Continued work will be aimed at developing new synthesis and coating techniques to achieve a thin, uniform coating over the entire surface of the foam. This will be followed by evaluation of thermal management during abuse testing.

The second cathode investigated is comprised of elemental sulfur with copper sulfide as the conductive additive. Others are using carbon black as the additive, but the electrochemical activity and high conductivity of the copper sulfides more than compensate for the added weight. Although tests of these materials fabricated as thin films were promising, significant challenges remain for the design and fabrication of a composite cathode with good structural stability and higher capacity. Continued work on this cathode has been deferred while issues with the lithium anode and electrolyte are addressed.

Investigation of the interface instabilities for the metallic lithium anode is the major new thrust of this project. For electric vehicle lithium-sulfur batteries, the lithium anode must accommodate stripping and plating of several tens of micrometers of lithium in each cycle, at moderate rates. Invariably, the lithium interface with the electrolyte roughens, leading to lost capacity, battery failure, or dangerous reactions. Several years ago, ORNL developed a thin-film solid electrolyte, known as Lipon. This electrolyte forms a stable interface with lithium metal and is quite robust in all solid-state microbatteries. In collaboration with researchers at Hydro Quebec, Lipon films will be assembled with other electrolyte materials in order to stabilize the lithium anode for larger-scale batteries. As part of this effort, new techniques for observing and characterizing the roughening lithium interface will be developed.

High Temperature Materials Laboratory

Lubrication Challenges for the Hydrogen-Fueled Internal Combustion Engine

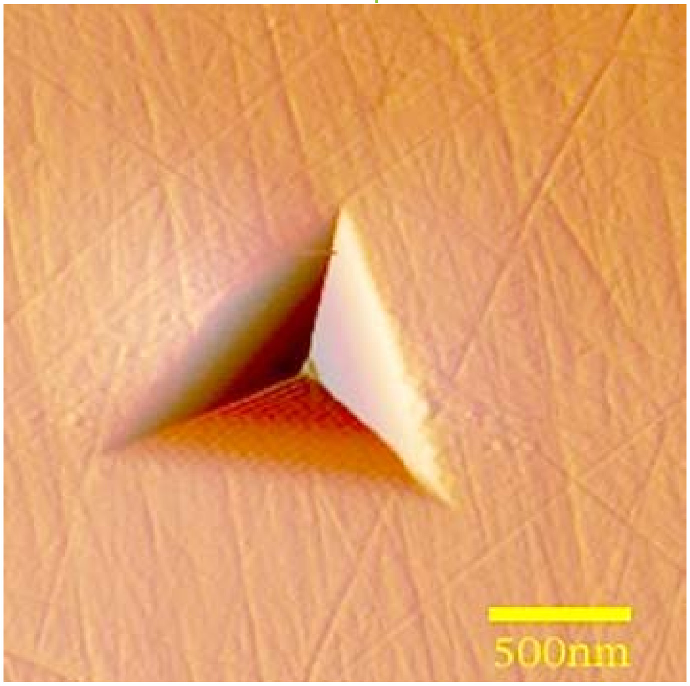

Figure 1. *A 'negative image' of the faceted diamond tip is replicated on this steel surface. The tip can be scanned to generate a surface map or used as a mechanical properties microprobe.*

Background

The use of hydrogen as a primary fuel for internal combustion engines (ICEs) presents numerous materials challenges. In liquid-fueled engines, the fuel itself provides a measure of lubrication for certain moving parts in the fuel injection system. In the case of hydrogen fuel (where there is no liquid to lubricate parts), however, maintaining adequately low friction and wear is problematic.

Oak Ridge National Laboratory (ORNL) staff (L. Reister and P. Blau) worked collaboratively with Pacific Northwest National Laboratory (PNNL) (J. Holbery) through the High Temperature Materials Laboratory User Program to characterize changes in the structure and properties of sliding surfaces of fuel injectors that were exposed to pressurized hydrogen gas.

The steel fuel injectors were first exposed to pressurized hydrogen for two days in a special autoclave at PNNL. They were then sectioned and brought to ORNL for nanoscale indentation and friction measurements. These tests, and surface topography analysis, were performed on a Hysitron Triboindenter™ in the Friction, Wear, and Machinability User Center.

Technology

The results of this project revealed that exposure to hydrogen environment can change the composition and structure of surfaces of fuel injector plungers sufficiently

Benefits

- Elucidation of technical and scientific challenges of hydrogen internal combustion engines.
- Better understanding of tribophysics of hydrogen exposure in internal combustion engines.

to alter their frictional characteristics. A method had to be developed for mounting the fuel injector parts so that the cylindrical inner bore can be probed with the measuring instrument. Profile scans and nano-scale indentation experiments revealed that friction and surface morphology were indeed affected by hydrogen exposure.

In some cases, the friction was lowered; but in multi-pass experiments, the friction rose.

Tiny hydride crystallites (100 nm to 5 µm across) were detected on the surface of the steel and may play a role in this behavior.

Status

Having established that hydrogen exposure can alter the friction and microstructure of fuel injectors, additional work is being planned to better elucidate the tribophysics of hydrogen exposure and its implications for enabling the technology of hydrogen-fueled automotive engines.

PNNL is working with commercial manufacturers of fuel injectors, but additional research is needed before specific engineering changes can be suggested in regard to the materials, the lubrication methodology, or the injector designs. Thus, further commercialization of new injector technology must be viewed as a longer-term outcome of this preliminary work.

In addition, results of this research were presented at a symposium on "Materials for a Hydrogen Economy," The Metallurgical Society, Pittsburgh, 2005.

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A Strong Energy Portfolio for a Strong America

Energy efficiency and clean, renewable energy will mean a stronger economy, a cleaner environment, and greater energy independence for America. Working with a wide array of state, community, industry, and university partners, the U.S. Department of Energy's Office of Energy Efficiency and Renewable Energy invests in a diverse portfolio of energy technologies.

High Temperature Materials Laboratory

Magnesium for Heavy Truck Applications

Background

Lighter-weight materials are being explored to increase the fuel efficiency of Class 8 trucks by replacing their heavier counterparts. A carbon fiber/magnesium composite, for example, is one-third the weight of aluminum. With this in mind, GS Engineering and Oshkosh Truck Corporation are part of a team that is developing truck components from magnesium metal matrix composite (MgMMC) materials. Such materials are prepared using a direct "squeeze casting" technique, in which carbon fiber performs are infiltrated with Mg.

However, in order to transfer MgMMC materials to vehicle component designs, their properties must first be understood. Thus it is important to know the interfacial reactions that take place at the fiber and Mg interface of the composite.

Technology

Research at the Oak Ridge National Laboratory (ORNL) has aided in the understanding of the reactions and effects of the reinforcements in the MgMMC. The microstructure of a carbon fiber-reinforced Mg alloy matrix (AZ91D) composite was characterized at the High Temperature Materials Laboratory (HTML) with the Phi 680 scanning Auger Nanoprobe (SAN). This instrument uses an electron beam in scanning mode to eject low energy electrons from the surface of the composite. The electrons can then by analyzed with a spectrometer to identify the chemical elements present in the composite's upper surface layers.

A high resolution secondary electron image of a polished sample (Figure 1) shows the morphology of the carbon fibers in the Mg alloy matrix. It also displays the presence of a reaction layer at the interface. The numbered spots on the figure indicate the locations and sizes of areas that were analyzed for elemental composition.

Electron spectra (displayed on the following page, in Figure 2), were collected from the analysis points to identify the elements present in the various phases of the microstructure.

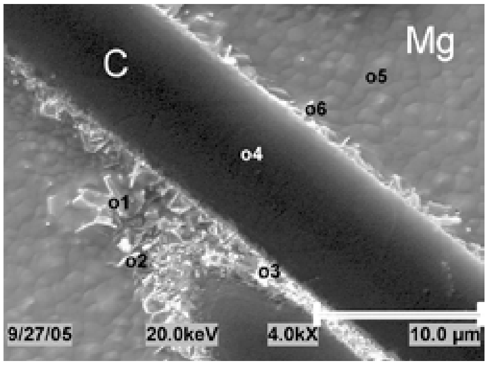

Figure 1. *A high resolution secondary electron image of a polished sample of the composite.*

Benefits

- The materials characterization at HTML provided useful data on the properties of MgMMC materials, which will help enable researchers to improve these materials for truck component design.
- Improved Mg alloy composite materials will contribute significantly to heavy truck weight reductions, therefore improving fuel economy.

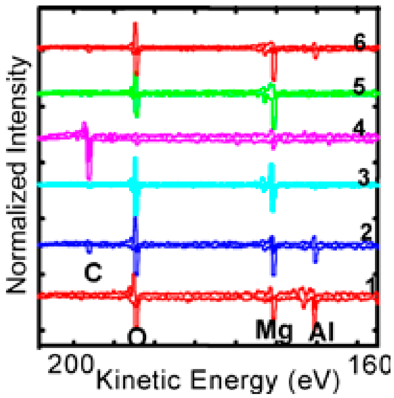

Figure 2.

of the locations of these various elements (Figure 3) showed the interface phase to be oxide rich.

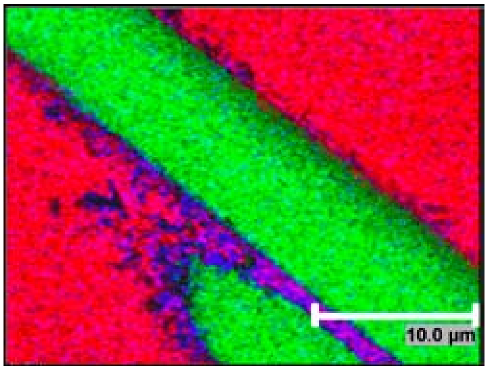

Figure 3.

Fiber cross sections (Figure 4) also show the reaction phase at the fiber-alloy interface.

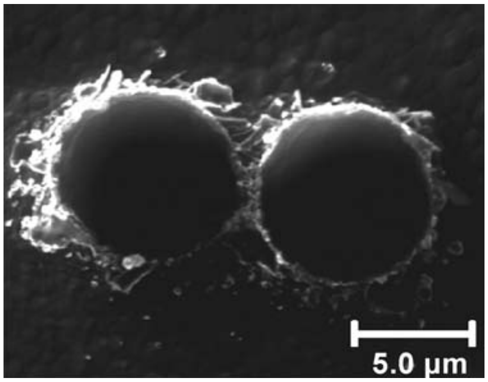

Figure 4.

Based on the SAN analysis, the interface oxide appears to be aluminum-rich (Figure 5). A significant diffusion of Mg into the carbon fiber was also revealed.

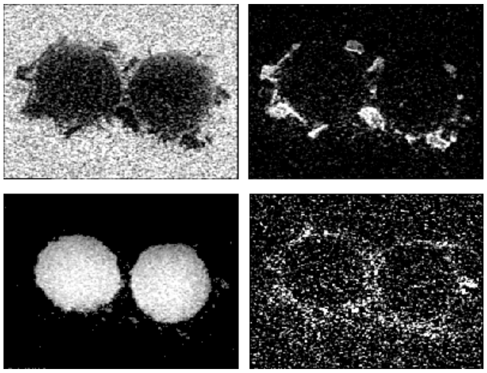

Figure 5.

Status

The results obtained in this project are immeasurable in their value to understanding how to improve MgMMC materials for truck component design. This materials characterization will provide direction for future MgMMC materials use, and because they are significantly lighter-weight, their implementation in heavy trucks will help improve fuel economy.

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High Temperature Materials Laboratory

Non-contact Weld Inspection in Ford Chicago Assembly Plant

Background

To reduce the overall weight of automobiles, U.S. car designers use steel sheets that have been stamped and welded in various parts of the body structure. In fact, most structural components in vehicles are held together by either resistance spot welds (RSWs) or laser welds (LWs). A survey by the U.S. Council for Automotive Research (USCAR) Nondestructive Evaluation (NDE) committee indicated that there is currently no in-line, nondestructive, weld inspection technology used by U.S. vehicle manufacturers.

Many of the current NDE techniques are post mortem. A labor-intensive, manual teardown inspection is performed every shift to determine weld quality, and in many cases, there can be a significant delay from the time a weld is produced to the time the same weld is inspected. For high-volume auto assembly production, the delay between welding and inspection could result in hundreds or even thousands of out-of-tolerance welded parts being made before detection.

In addition, most of these techniques are contact methods. These have proven difficult to implement, and automakers have realized the importance in developing a reliable, non-contact NDE weld inspection technique. Such a technique would be beneficial by improving inspection reliability and efficiency.

HTML's Thermography and Thermophysical Properties User Center houses state-of-the-art infrared (IR) cameras that can take hundreds of images per second with a temperature resolution of just over one hundredth of a degree. The instant imaging results in temperature maps that can produce visual results of any heat-related process. Even more important for this project, infrared imaging can detect the thermal radiation of an object in a non-contact fashion.

When two metal sheets are joined by a weld (lap joint), the weld provides a heat conduction path from one sheet to another.

Figure 1. *Set-up of an infrared imaging system for laser weld inspection at the Ford assembly line.*

Benefits

- Reduced number of labor-intensive tear-down inspections.
- Improved quality control and inspection reliability.
- Potential real-time monitoring of the laser weld process.

Based on this fact, IR imaging can be used to inspect welds. Two primary methods have been used for weld inspections: heat sink and heat leak. For the Ford project, the heat leak method was used for both RSWs and LWs.

Technology

The IR camera is a portable system and can be operated from a laptop computer. The non-contact feature made it possible to conduct testing at the assembly plant without interrupting or interfering with the production process.

In addition, IR imaging provided a potential for real time monitoring of the laser weld process. It has already been demonstrated at the Oak Ridge National Laboratory (ORNL) that the IR camera can capture defects during the welding process. The welding heat and temperature distribution can then be used to monitor and control the process.

In the Ford project, 12 vehicles were inspected within a 2-hour period for LWs. The IR imaging system confirmed that one particular weld stitch was having quality problems. Some potential problem areas for spot welds were identified. Some "cold" welds were found on areas when no heat was coming through after the opposite side was heated with hot air. The IR imaging system was able to identify a consistent lack-of-fusion weld in multiple vehicles.

Status

Further work on the IR imaging system is ongoing. ORNL is working closely with U.S. auto manufacturers to ensure that the R&D of this technology is closely aligned with their needs. This will provide a clear path to commercialization in the future.

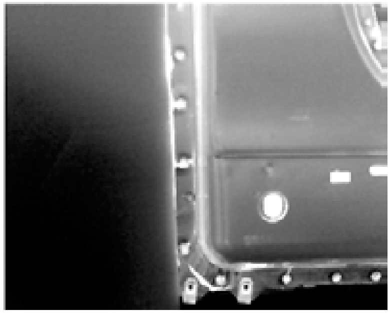

Figure 2. *IR image of four welds before heating.*

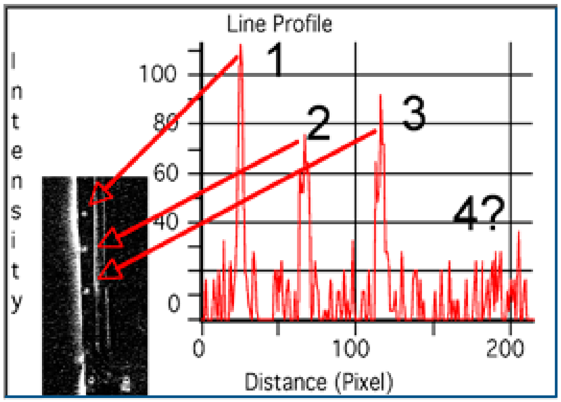

Figure 3. *Heat came through three of the four welds, indicating lack of fusion on the fourth.*

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High Temperature Materials Laboratory

Residual Stress Mapping of High Strength Steel Weldments to Improve Fatigue Life

Background

Attempts to improve fuel economy in both on-highway and off-highway vehicles are increasing due to oil shortages and environmental factors. Reducing the weight of vehicles can contribute to improved fuel economy. However, designing and producing lighter weight structures for these vehicles with high strength materials is limited by the low fatigue strength of welded joints.

High tensile residual stresses are usually formed in high-strength steel welds. High tensile residual stresses accelerate fatigue crack propagation and reduce weld fatigue life, which makes developing fatigue-resistant welds a major technical barrier.

A systematic approach was developed by Caterpillar to improve the fatigue life of a welded joint by 10 times and to reduce energy use by 25 percent. The approach involved developing special welding wires and evaluating the weld process with the goal of introducing compressive residual stress at the weld toe of high strength steel welds. The residual stress facilities at the High Temperature Materials Laboratory (HTML) were used by Caterpillar to characterize the residual stresses at critical locations in the vicinity of their experimental welds.

Figure 1. High strength welded steel sample mounted and ready for stress mapping at the new neutron residual stress mapping facility.

Technology

Diffraction is used to probe the crystal structure of materials. Specifically, the spacing between planes of atoms can be accurately measured. Applied or residual forces pull or squeeze

Benefits

- Significant reduction of detrimental tensile residual stresses improves fatigue life.
- Increased use of high strength steel enables reduced vehicle weight.

the crystal structure, changing the spacing of these planes. This change can be measured and converted into a residual stress. Diffraction can be accomplished with X-rays and neutrons, which provide information from the surface and bulk of a material, respectively. Measurement at many locations within the specimen and its surface leads to maps of residual stresses. These stress maps are used for life prediction and model validation.

Neutron strain mapping was performed using the new Neutron Residual Stress Mapping Facility operated by the HTML at the High Flux Isotope Reactor. An advanced monochromator delivers a high flux of neutrons to the sample. Computer controlled stress mappings along lines two and three (see Figure 2) were collected for three different weld metals.

Residual stresses along line 1 of Figure 2 were mapped starting from the weld toe out 5 mm

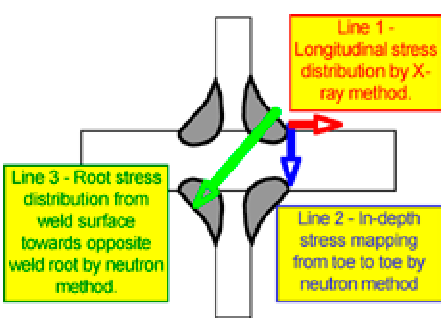

Figure 2.

using HTML's large specimen X-ray diffraction facility with computer controlled specimen positioning. The X-ray system consists of a portable X-ray stress analyzer mounted overhead to a gantry which forms the frame for a 15 × 8.2 × 9.2 ft (L × W × H) shielded enclosure. This setup can accommodate small and large samples up to 250 lb.

Status

The measured residual stresses for the three types of welded joints investigated are more compressive than in the conventional weld. The stresses are consistent with those from the simulation, that is, tensile residual stress at weld toe with conventional welding wire and compressive residual stress at weld toe with special welding wires.

The predicted fatigue life using a two-stage crack growth model considering the effect of compressive residual stress with special welding wire welds are in reasonable agreement with the high end of fatigue test results, which show more than 10 times the fatigue life improvement in high strength steel welded joints.

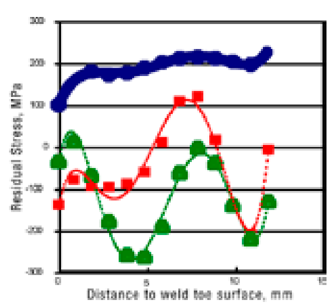

Figure 3. *Measured residual stress maps along line 2 in the direction perpendicular to the weld line for the conventional weld (blue) and special welding wires (red and green).*

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Advanced Power Electronics

Dual Integrated Inverter for Automotive Applications

Background

There are several drawbacks associated with conventional engine, belt-driven compressors for heating, ventilating, and air-conditioning (HVAC):

- Low operational efficiencies: The compressor speed is determined by the engine speed and cannot be adjusted according to the cooling/heating requirements.
- Inflexible packaging: The HVAC location for installation is restricted to the accessory drive side of the engine.
- Frequent maintenance requirements: Because of the difficulty in completely sealing the rotating shaft, there is possible belt breakage and refrigerant leakage into the atmosphere.

In order to overcome these problems, it is more ideal to use electric motor-driven compressors in automobiles with 42V power nets and high-voltage buses, such as hybrid electric vehicles. An electric drive allows the air conditioner output to be matched to the vehicle air conditioning load.

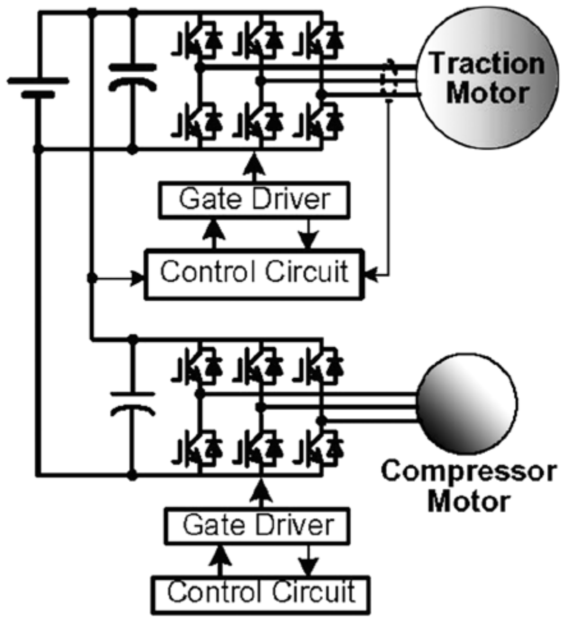

Figure 1. *Conventional configuration employing two three-phase drives.*

Additionally, the cost and volume of the compressor drive can be reduced by integrating the two inverters necessary for the traction drive and the compressor motor. As automakers move toward electronic drives using two-phase motors, requirements for the inverters will be sought to ensure that R&D activities are closely aligned with market needs.

Benefits

- Eliminates the use of belts, abating the associated maintenance.
- Reduces cost and size of the compressor drive.
- Increases efficiency and reduces fuel consumption.
- Allows matching of air conditioner output to load.

Technology

Researchers at the Oak Ridge National Laboratory used a two-phase motor to replace the conventional three-phase motor, eliminating one phase leg. The design of the integrated inverter reduces part count by sharing switching devices, DC bus filter capacitors, gate drive power supplies, and control circuitry. In addition, each motor's torque-producing currents and speeds can be controlled independently.

The new design, shown in Figure 2, utilizes component sharing and results in a five-leg inverter. The inverter can drive a three-phase traction motor and a two-phase compressor motor with the benefits of lower cost, reduced volume, and increased efficiency and reliability.

Status

The novel system eliminates the belts and associated maintenance required in the previous one. The number of switches and other components is reduced by 33 percent, reducing the cost and size of the compressor drive. Increased efficiency and reduced fuel consumption, as well as the ability to match output load, result with the new design.

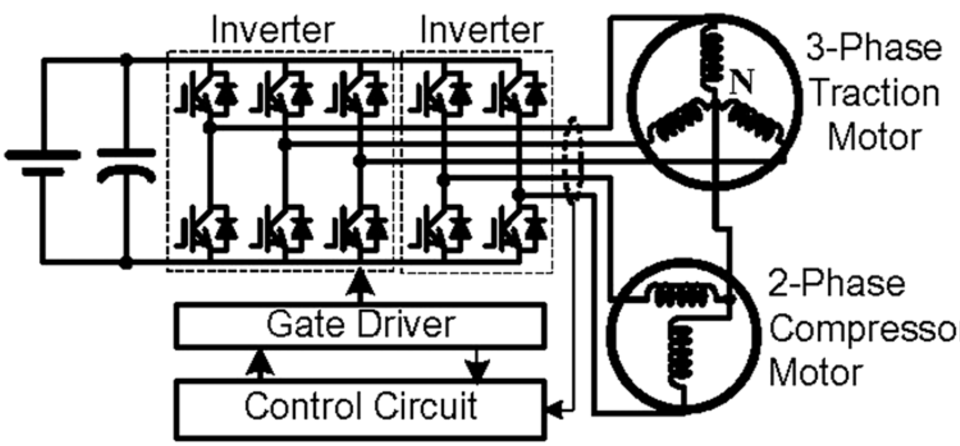

Figure 2. *Dual integrated inverter for traction and compressor drives*

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Advanced Power Electronics

Internal Permanent Magnet Reluctance Machine Utilizing Brushless Field Excitation

Background

Permanent magnet (PM) motors are quickly gaining acceptance as the "electric motor of choice" for hybrid and electric vehicle traction drives. This technology offers a higher power density motor with enhanced performance benefits over other motor types that have been previously considered for traction drive applications. However, technological and economic barriers still exist for this emerging technology.

Field weakening techniques are necessary to expand the speed range of the system. These often add complexity and increase the cost of the inverter. Additional techniques are necessary to enhance the starting torque. As motor speeds increase, the higher back EMF creates the need for boost converters to produce higher bus voltage, also adding to costs.

Technology

Through the addition of external excitation coils, the field of the motor can be both weakened and enhanced to negate these barriers. In a conventional PM machine, the air-gap flux produced by the magnets is fixed; it is difficult to enhance the air-gap flux density due to limitations of the permanent magnets in a series-magnet circuit. However, the air-gap flux density can be weakened by using field weakening techniques.

Researchers at the Oak Ridge National Laboratory (ORNL) have developed a technology that uses external excitation coils to enhance and weaken the air-gap flux density. This technology makes the ability to manipulate the field utilizing costly boost converters in the system unnecessary.

The potential exists for using weaker, less costly permanent

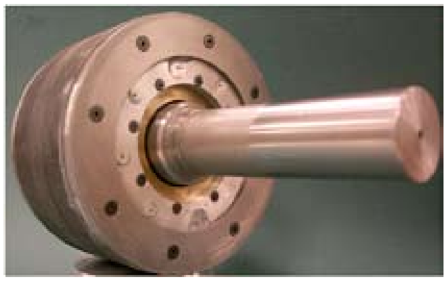

Figure 1. A permanent magnet motor.

Benefits

- Increases power density of the system.
- Decreases system size and weight.
- Eliminates the need for a boost converter in the system.
- Increases the reluctance torque component, resulting in a higher total torque output.
- Increases flux density in the motor.
- Reduces core losses at higher speeds.

magnets in the motor, resulting in additional significant cost savings. Minimal control circuitry and power is required to implement this technology.

Status

This effort is still in its early stages; the current design is being optimized. ORNL is working closely with U.S. auto manufacturers to ensure that the R&D of this technology is closely aligned with industry needs, providing a clear path to commercialization in the future.

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Advanced Power Electronics

ORNL Floating Loop Integrated Hybrid Electric Vehicle Cooling System

Background

It is of continuing interest in the hybrid electric vehicle arena to increase power density and decrease weight and volume in the hybrid drive train. Vehicle cooling systems range across several types of systems and fluids, such as radiator coolant (water/ethylene glycol), transmission fluid (oil), and passenger air conditioning refrigerant (presently R134a). Hybrid drive trains on the market today are using radiator coolant loops to cool the power electronics and traction motors. In order to enable power densities to continue increasing and reliability to continue improving, the need for efficient, compact cooling systems is growing.

Technology

The Oak Ridge National Laboratory (ORNL) floating loop integrates the traction drive cooling system with the passenger air conditioning (A/C) system and shares some components of the passenger A/C system (i.e. piping, refrigerant, and condenser). This system provides the effective two-phase cooling directly for the inverter and motor. The integration of this floating loop into the A/C system eliminates the need for a separate piping system, compressor, and heat exchanger. The integration only adds a small pump to promote flow through the new section of the refrigerant system.

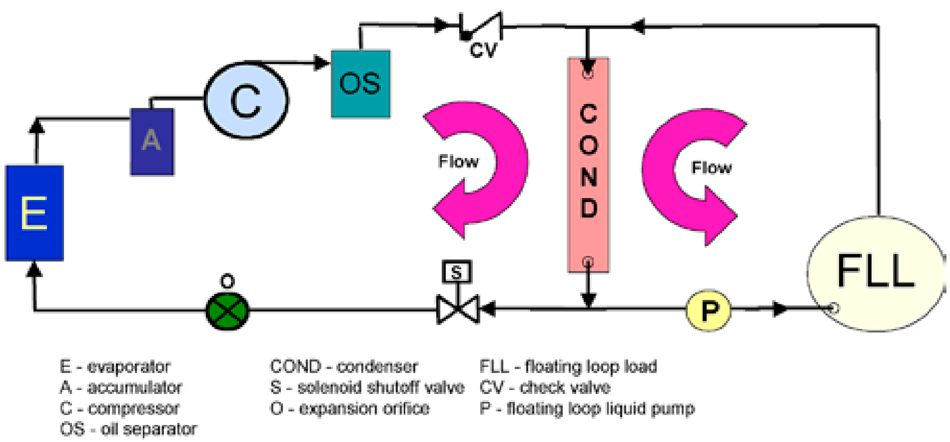

Figure 1. *R134a integrated cooling system with floating loop*

Although sharing some components and piping, the cooling system remains operationally independent from the A/C system, allowing the subsystems to operate together or alone. The system provides two-phase cooling at 50 to 60°C, where traction drive heat is rejected to ambient through he refrigerant to surrounding air.

Benefits

- Enables higher power density.
- Improves reliability and lifetime by lowering operating temperatures for the electronics.
- Allows increased silicon chip power throughput.
- Shares existing components under the hood of the vehicle.

Status

Testing at ORNL has shown the cooling system to function well as an integrated part of the existing A/C system, and the floating loop system has demonstrated a coefficient of performance (COP) greater than 40 for the floating loop segment.

While work on this effort is still in its early stages, the current design is being optimized. ORNL is working closely with U.S. auto manufacturers to ensure that the R&D of this technology is closely aligned with industry needs, providing a clear path to commercialization in the future.

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Advanced Power Electronics

Wide Bandgap Materials

Background

Power devices used in traction applications must be able to handle extreme environments which include a wide range of operating temperatures. Because of their physical properties, silicon (Si) devices have generally reached their operating temperature limits in such conditions.

Silicon carbide (SiC) has been identified as a material with the potential to replace Si in power devices. SiC-based devices are capable of operating at high voltages, high frequencies, and at higher junction temperatures. It is projected that significant reductions in the weight and size of SiC power electronics as well as an increase in operational efficiency can be achieved through utilization of this semiconductor technology.

Technology

The Oak Ridge National Laboratory (ORNL) has been assessing the impact of replacing Si power devices in transportation applications with SiC-based power devices.

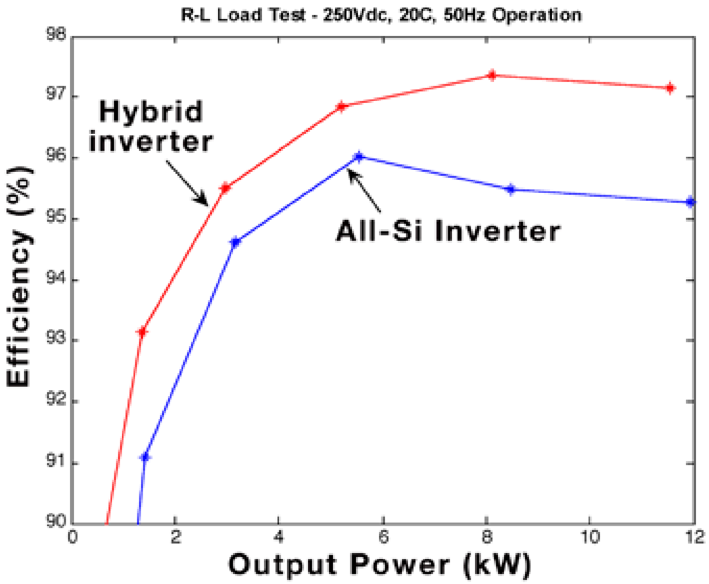

Figure 1. *Efficiency comparison of a 55-kW Si IGBT-SiC Schottky diode and a similarly rated all-Si inverter.*

The use of SiC is projected to significantly reduce the weight and size of current power electronics, as well as increase operational efficiency.

Extensive dynamometer and inductive load testing of this hybrid inverter showed a reduction of up to 33.6 percent in inverter losses. When SiC main switches also replace their Si counterparts, inverter losses are expected to be reduced by up to 65 percent.

Benefits

- Enables higher power density.
- Improves reliability and lifetime by lowering operating temperatures for the electronics.
- Allows increased silicon chip power throughput.
- Shares existing components under the hood of the vehicle.

Status

Recently, ORNL collaborated with Cree and Semikron to build a 55 kW Si IGBT and SiC Schottky diode inverter. Schottky diodes are the only SiC devices that are presently commercially available and are provided by only a handful of manufacturers. Several companies and universities are developing other SiC and gallium nitride power electronics devices, but have not yet introduced commercial products for JFETs, IGBTs, or MOSFETs. SiC device manufacturers are expected to commercialize SiC JFETs and MOSFETs.

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Fuels, Engines, and Emissions

Elucidating Lean NO_x Trap Fundamentals via Intra-Catalyst Diagnostics

Background

An effective catalyst-based aftertreatment will be needed to meet upcoming U.S. EPA emission standards for diesel nitrogen oxide (NO_x) emissions. Three-way catalysts are already well established for gasoline NO_x abatement, but these are not effective in the oxygen-rich diesel exhaust. In order to overcome this issue, the lean NO_x trap (LNT) combines the NO_x storage function with the three-way catalyst.

The LNT stores NO_x under normal lean operation (the storage step) and releases and reduces the stored NO_x during short, periodic, rich excursions (regeneration step). Successful implementation of this technology will require a highly efficient engine-LNT system configuration and control. This will allow the diesel engine to meet EPA standards with minimum fuel penalty associated with regeneration. Thus, a fundamental understanding of LNT process details is critical.

Knowledge of how a reductant evolves and is utilized inside a working catalyst channel during LNT regeneration will be crucial to understanding the process. In addition, the intrinsically transient and integral nature of LNT devices makes the use of spatially and temporally resolved diagnostics highly desirable for elucidating complex LNT regeneration chemistry.

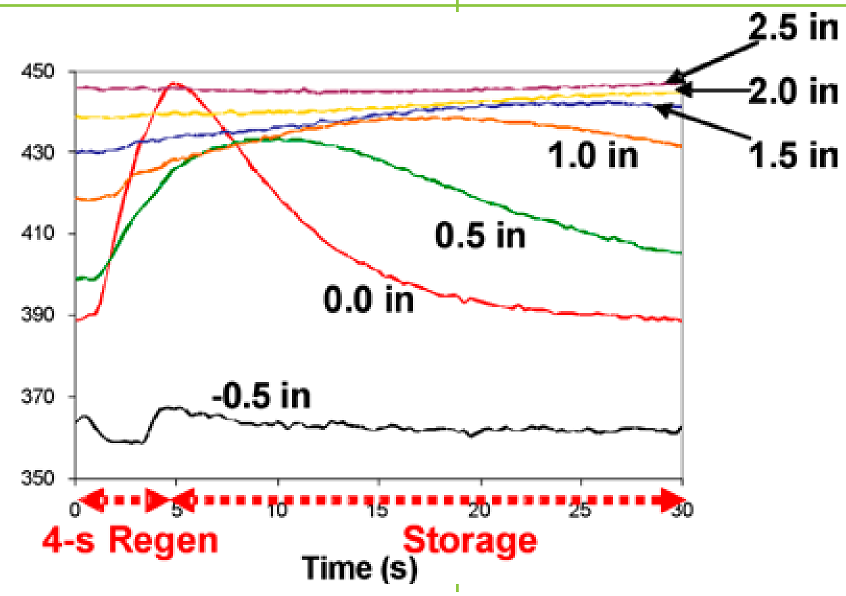

Figure 1. *NO_x, H_2, H_2O, and temperature transients occurring during regeneration of a 3-in.-long LNT.*

Technology

In this project, the Oak Ridge National Laboratory (ORNL) team developed and applied two microprobe techniques to characterize in situ chemical and thermal processes occurring during LNT regeneration: spatially resolved capillary inlet

Benefits

- Provides chemistry details that are difficult to obtain via conventional "catalyst-outlet-only" analytical tools.
- Facilitates development of improved LNT formulations and predictive kinetic models.
- SpaciMS and phosphor thermography proved to be efficient tools in validating sub-system- and system-level kinetic modeling.
- Facilitates fuel-efficient system configuration and engine control strategy development.

mass spectrometry (SpaciMS), and fiber-coupled phosphor thermography.

SpaciMS utilizes capillaries for minimally invasive in situ gas sampling from within catalyst monolith channels during catalyst operation. The sample gas (including H_2, H_2O, NO_X, O_2, CO_2, H_2S_2, SO_2, and various hydrocarbons) is collected by capillaries (180 µm OD, 10 µL/min) and fed to a mass spectrometer for broad species analysis. Currently, temporal resolutions of 10 to 1 Hz have been achieved.

The phosphor thermography instrument is based on a phosphor-tipped ca. 200-µm OD optical fiber. Through remote excitation, the phosphor tip emits fluorescence detected through the fiber (the decay rate of fluorescence is indicative of the phosphor temperature). Non-conductive optical fibers are minimally invasive and eliminate conductive broadening of spatially distinct thermal gradients as is characteristic of thermocouples.

Status

By translating the SpaciMS and phosphor thermography probes inside LNT monolith channels, dynamic species and temperature distributions throughout an LNT device could be resolved and led to new insights regarding LNT regeneration with CO (carbon monoxide) reductant:

- The network and sequence of regeneration reactions:
  - residual O_2 depletion at the catalyst front end;
  - highly efficient primary NO_X release and reduction;
  - slower and minor secondary NO_x release and reduction; and
  - H_2 formation via a water-gas shift and NH_3 production during the secondary NO_X release and reduction.
- Poor LNT performance at low temperature due to CO poisoning Pt sites.
- Occurrence of exotherms and heat transfer:
  - a high exotherm at the catalyst front due to CO oxidation;
  - smaller but more axially extended NO_X-attributable exotherms; and
  - slow heat dissipation and resulting temperature increase during the subsequent storage phase.

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Fuels, Engines, and Emissions

In-Cylinder Hydrogen Generation May Enhance Catalyst Function

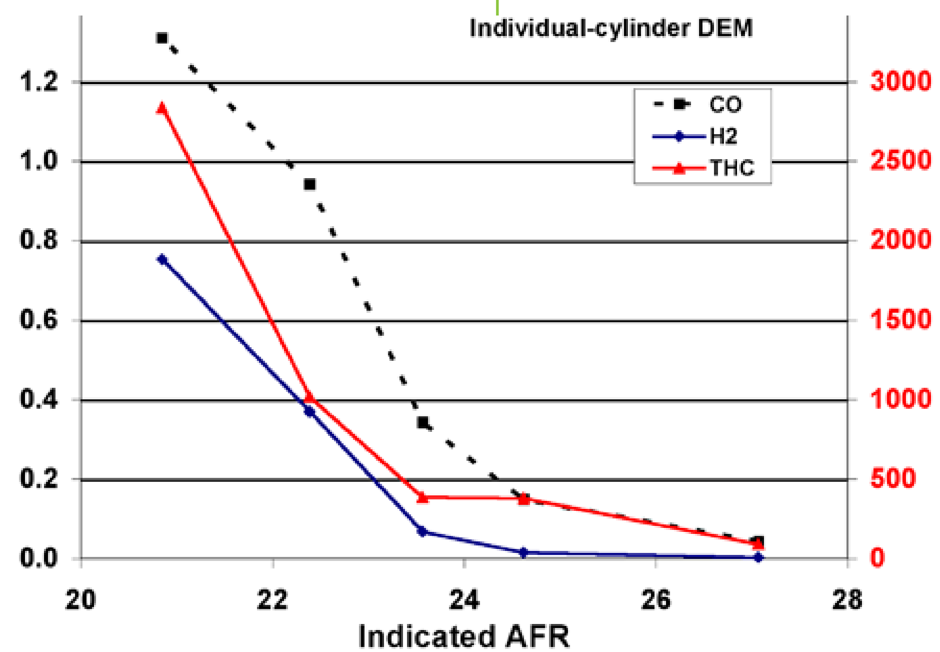

Figure 1. Measured levels of H_2, CO, and total HC in engine-out exhaust at various net air-fuel ratios using an individual-cylinder delayed and extended main (DEM) fuel injection strategy.

Background

New low temperature combustion (LTC) regimes are being investigated as a means to improve the efficiency of diesel engines. The lower engine-out nitrogen oxide (NO_x) emissions in LTC modes can remove some burden from post-combustion emissions controls and reduce the fuel penalty associated with NO_x reduction. In addition, new combustion regimes that will improve brake-specific fuel consumption are being sought.

However, while these combustion regimes will be exploited to whatever extent possible in future production engines, diesels are still expected to run in the more conventional modes at certain operating conditions. The wide range of operating conditions provides a challenging environment for the aftertreatment system. Multi-mode operation of the engine will almost certainly require a multi-mode aftertreatment system.

While lean NO_x trap (LNT) and urea SCR (selective catalytic reduction) technologies show great promise in reducing NO_x under conventional diesel combustion conditions, the lighter-load, low-NO_x LTC regimes may require different catalyst technology. Treatment of HC (hydrocarbon) and CO (carbon monoxide) emissions during LTC is also a concern. Because of the relatively high HC to NO_x ratio in LTC modes, HC SCR may be an attractive option to augment the LNT or urea SCR systems. In recent

Benefits

- Better understanding of low-temperature combustion regimes.
- Enables efficient, clean diesel engines in light-duty applications.

H_2 in the feedgas. On-board fuel reformers are being researched as a potential way to generate H_2 for the aftertreatment system.

In a previous LNT research activity, engineers at ORNL developed regenerating strategies for LNTs using a rapid prototype engine controller. While the diesel engine normally runs fuel lean [with an air to fuel ratio (AFR) typically much greater then 14.5], the LNT requires a periodic rich excursion, a short duration pulse in which the AFR dips below 14.5. The rich, or reducing, conditions allow release and reduction of the stored NO_x on the LNT. One strategy for this rich excursion is the "delayed and extended main" or DEM, in which the main fuel pulse is delayed in crank angle time and extended into the rich regime.

Technology

This project's goal was to leverage existing combustion and aftertreatment R&D at ORNL and collaborate with industry partners to develop and characterize advanced catalysts. The project investigated a means of generating H_2 and other reformate products in the engine cylinders.

Recent publications have shown that H_2 can promote the catalytic reduction of NO_x in HC-SCR catalysts operating in the lean regime. With this knowledge, researchers at ORNL modified the DEM strategy to investigate reformate production under net-lean conditions. The investigated approach makes use of individual cylinder control. The "individual cylinder DEM strategy" commands one cylinder to run rich while the other three run lean. The rich cylinder is indexed from one cylinder to the next with only one cylinder in the rich regime at any given time.

Status

With the individual cylinder approach, researchers have proved that up to 0.8% H_2, over 1% CO, and 3,000 ppm (parts per million) HC can be produced under net lean conditions with over 9% O_2 still present in the exhaust. Preliminary experiments have shown that this unusual combustion approach can accelerate catalyst light-off. Future experiments will investigate the promotional effects of these exhaust species on catalyst function.

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Fuels, Engines, and Emissions

Low Temperature Combustion for use as a Diesel Engine Lean NO_x Trap Regeneration Strategy

Background

As part of the Department of Energy's strategy to reduce petroleum imports and improve energy security, the FreedomCAR and Vehicle Technologies Program researches technologies that will enable more efficient diesel engines to meet EPA's emissions regulations for nitrogen oxides (NO_x). Control of NO_x emissions is critical for enabling clean, fuel-efficient diesel engines. The use of lean NO_x trap (LNT) catalysts is an active focus for diesel engine NO_x control. LNT performance must be better understood in order to improve the control of NO_x emissions.

An LNT catalyst will absorb NO_x during normal lean operation, typical of diesel engines. These catalysts are very effective, but they must be regenerated as often as every 30 to 90 seconds. Regeneration is accomplished by exposing the LNT to rich exhaust gas which causes the LNT to release the NO_x and chemically reduce it to harmless nitrogen.

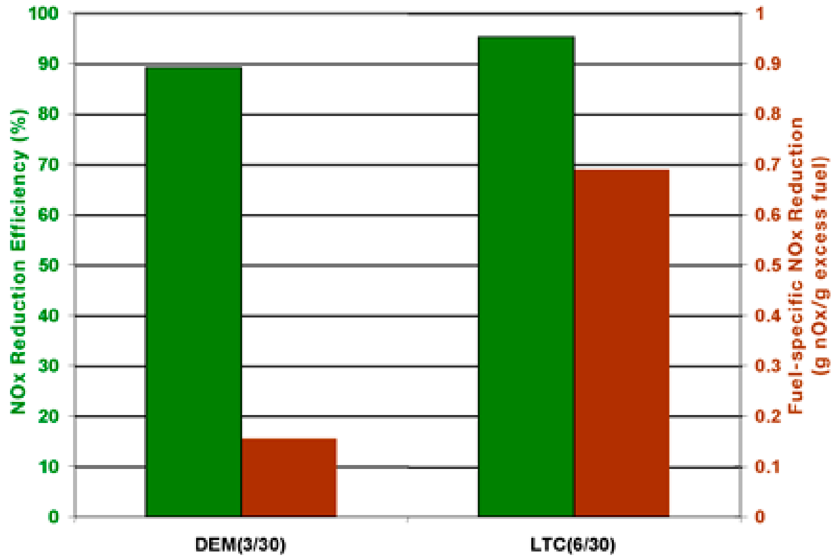

Figure 1. *Comparison of strategies for NO_x reduction and fuel utilization.*

Technology

Researchers at the Oak Ridge National Laboratory (ORNL) are using advanced instrumentation and measurement methods to develop and characterize different control strategies for maintaining peak catalyst efficiency. Using a modern 1.7-liter Mercedes common-rail, turbocharged diesel engine with

Benefits

- The low fuel consumption for LTC regeneration yields superior fuel specific NO_x reduction.
- Preliminary data indicates potential for catalyst performance equivalent to other strategies, but with five times more efficient fuel utilization.

full electronic control, ORNL researchers have developed several strategies for LNT regeneration. These strategies typically use throttling, excess fuel, increased EGR, or some combination to induce the rich operation necessary for LNT regeneration.

Under certain operating conditions extreme amounts of EGR (>50%) can induce what is referred to as low temperature combustion (LTC). LTC operation is characterized by simultaneous low NO_x and low particulate matter (PM), which is highly desirable.

It has been found that with a nominal amount of excess fueling, rich LTC operation can be effectively used for LNT regeneration. For LTC regeneration, 50-55% EGR decreases the air to fuel ratio (AFR) to near stoichiometry, while a small amount of fuel is used to drive the engine rich. Because the required amount of excess fuel is much less than other strategies, LTC carries a greatly reduced fuel penalty.

Status

LTC regeneration has been shown to achieve comparable NO_x reduction when compared with other strategies, such as one that delays and extends the main fuel pulse (DEM) to induce rich operation. Comparing the DEM and LTC strategies on a fuel specific NO_x reduction basis (that is, grams of NO_x reduced per gram of excess fuel used) the LTC strategy utilizes fuel some five times more efficiently. The LTC strategy has great promise for contributing to the FCVT Program's low fuel penalty goals.

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Fuels, Engines, and Emissions

Stabilizing and Expanding HCCI Combustion with Spark Assist

Background

Gasoline engines are expected to dominate the U.S. passenger car market for at least the next decade. An improvement in the fuel efficiency of these engines would significantly reduce U.S. energy usage.

Homogeneous charge compression ignition (HCCI) in internal combustion engines is of considerable interest because of the potential reductions in nitrogen oxide (NO_x) emissions and fuel economy improvements resulting from unthrottled operation, faster heat release, and reduced heat transfer losses.

HCCI may not be sustainable under all conditions and loads in transportation applications. Thus, expanding the stable operating range and the ability to rapidly switch between HCCI and spark ignition combustion are the most important technical developments needed to achieve wide-spread HCCI utilization.

In addition, there are clearly many engine conditions under which HCCI is physically possible but marginally stable.

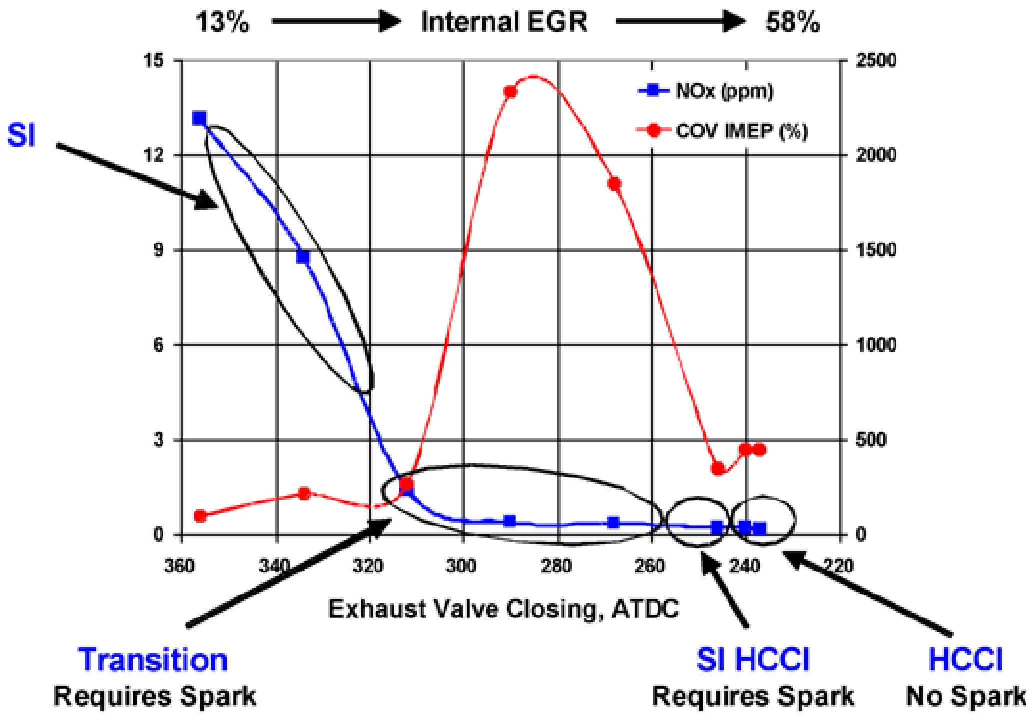

Figure 1. Stability and NO_x emissions during the transition from SI to HCCI combustion using internal EGR.

Because of this, the full potential cannot be realized until appropriate stabilizing strategies are developed to maximize the practical range of implementation.

Technology

The development of both combustion-mode switching and HCCI stabilization technologies requires that the fundamental nature of the transition between spark ignition (SI) and HCCI

Benefits

- Confirmed advantages of HCCI combustion as compared to unthrottled conventional operation.
- Enabled transitions to HCCI combustion and extended stable operating range.
- Identified and characterized existence of deterministic structure in cycle-to-cycle variations.
- Potential for development of control algorithms for expanding stable HCCI operation.

combustion be well understood, especially in the context of realistic engine conditions.

Oak Ridge National Laboratory (ORNL) researchers have mapped engine operation and stability for the transition between spark ignition and HCCI combustion modes on a single-cylinder engine. The instability appears to be low-dimensional. This suggests the possibility of developing on-line diagnostics and proactive control algorithms for expanding stable HCCI operation and improving transitions between conventional and HCCI modes.

Status

Commercial application of HCCI strategies will require advances over a broad range of technologies including combustion mode sensing (direct or virtual), combustion control, and mode transition control. ORNL is addressing these enabling technologies as a path to meeting DOE goals of improved emissions and efficiency. The results from of this activity are being shared with industry, universities, and other national laboratories. Examples include regular presentations to a multi-laboratory, multi-company working group on advanced engine combustion research and regular publications with the Society of Automotive Engineers and the Combustion Institute. ORNL also reports findings to industry stakeholders annually at both the Advanced Combustion and Emissions Program Merit Review.

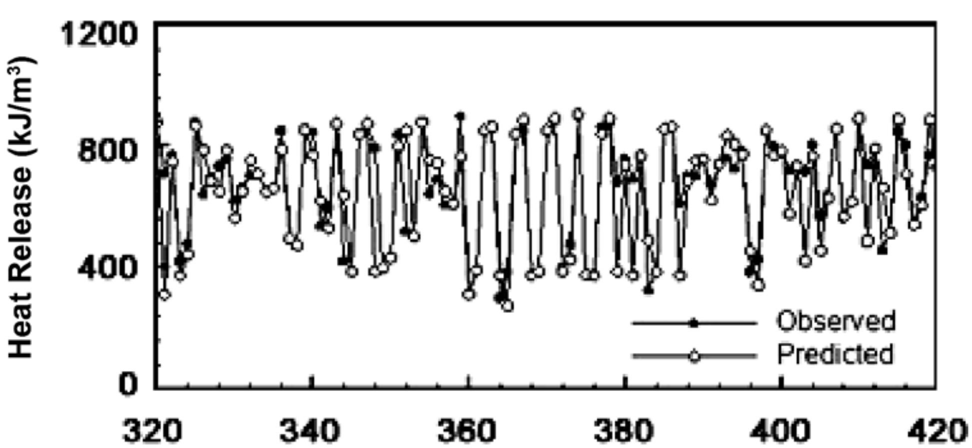

Figure 2. Example of experimentally observed and predicted heat release time series for SI-HCCI transition.

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Fuels, Engines, and Emissions

Understanding Particulate Formation Processes in High-Efficiency Clean Combustion (HECC)

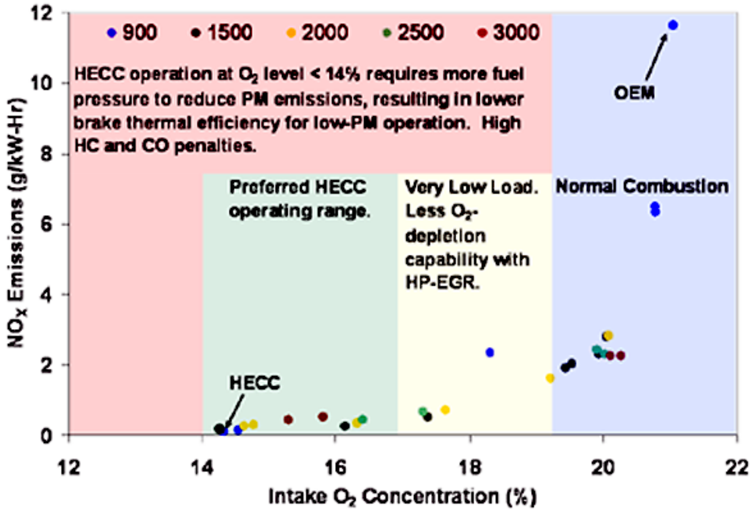

Figure 1. *Engine-out NO_x emissons at various engine rpm levels and intake oxygen concentrations.*

Background

Compression-ignition (CI, or diesel) engines have long been known for their relatively high efficiency compared with spark-ignition (SI) engines. However, conventional approaches to diesel combustion have been plagued by a trade-off between nitrogen oxide (NO_x) and particulate matter (PM) emissions. A strategy that reduced one pollutant typically increased the other.

Recent theoretical and experimental studies describe the existence of combustion regimes which exhibit simultaneous low NO_x and PM emissions. Utilization of these regimes in production vehicles offers the opportunity to reduce the performance requirements for aftertreatment technologies and improve overall engine system efficiency.

This project focuses on improving the performance of high-efficiency clean combustion (HECC) and on expanding the engine operating space where this combustion strategy can be utilized. Data gathered during this project can help further the understanding of pollutant formation processes

in near-production multi-cylinder engines. This understanding may lead to improved combustion models and engine designs.

Technology

Studies performed by Oak Ridge National Laboratory (ORNL) have shown that low-temperature combustion strategies produce particulate that contains a large fraction of soluble organic compounds

Benefits

- Increased understanding of the PM-formation processes in production-like multi-cylinder engines that operate in HECC and related combustion modes.
- Improved models for emissions control technologies to foster better integration between emissions control technologies and combustion strategies.
- Development of strategies for improving engine system efficiency through thermodynamic analysis of HECC and related combustion modes.

and, in some cases, significant increases in semi-volatile species. Increasing the fuel volatility may allow broader use of HECC and related combustion modes.

Combustion strategies that use EGR to displace O_2 in the fresh charge can cause semi-volatile compounds to partition from the gas phase to the particulate phase. This results in potentially important PM measurement issues in HECC and related combustion modes. In addition, low-O_2 modes increased the levels of gas-phase soot-precursor species that continue to participate in soot-formation processes through recirculation in the EGR gases.

Status

ORNL is participating with fourteen other organizations in a Memorandum of Understanding (MOU) on Advanced Engine Combustion Research. In addition to dissemination of study findings through publications, such as through the Society of Automotive Engineers and the Combustion Institute, ORNL reports results to the group twice each year. ORNL also reports findings to industry stakeholders annually at both the Advanced Combustion and Emissions Program Merit Review and the Fuels Technology Program Merit Review.

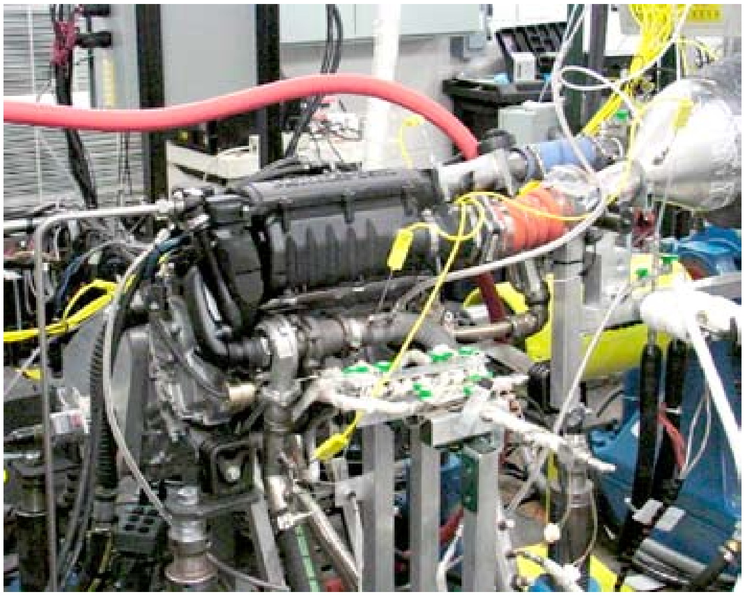

Figure 2. Photograph of Mercedes 1.7 liter engine installed in ORNL engine research cell 4.

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Automotive Lightweighting Materials

Carbon Fiber Systems Integration

Background

Because of their high stiffness, high strength, low mass, and low thermal expansion, carbon fiber reinforced polymer composites offer compelling benefits in automotive structures. They can significantly reduce vehicle weight and fuel demand. However, their widespread automotive use has been limited by high materials and processing cost. The selling cost of carbon fiber needs to be reduced to less than half of current prices to become cost-competitive with incumbent materials. Oak Ridge National Laboratory (ORNL) is leading a program to develop low cost carbon fiber technology that includes low cost raw materials and fiber conversion processes. The various developmental materials and conversion modules will be tested, refined, and integrated into a functional system in a modular test facility at ORNL. The test facility will include a subscale conventional modular pilot line that will be mated to advanced technology test modules for testing the latter. The conventional pilot line was recently acquired and installed at ORNL.

Figure 1. *Conventional, subscale, pilot carbon fiber conversion line installed at ORNL.*

Technology

ORNL is developing methods to rapidly and inexpensively stabilize, oxidize, carbonize, graphitize, and post-treat

Benefits

- Conversion processes under investigation will reduce time, space, and cost of producing carbon fibers.
- Pilot line will serve as a test bed for advanced technology modules.
- Pilot line will be used to test alternative precursors.

commercial grade carbon fibers made from polyacrylonitrile precursor. Advanced processing methods such as microwaves, plasma, infrared, ultraviolet, electron beam, and combinations thereof are under investigation. Additionally, lower cost precursors from other sources are also in development. The recently acquired pilot conversion line employs conventional thermal pyrolysis technology.

Status

ORNL is working with the Automotive Composites Consortium, as well as heavy truck OEMs and automotive/truck suppliers, to engage both existing and prospective carbon fiber manufacturers. Multiple carbon fiber manufacturers have participated in or contributed to the low cost carbon fiber program, but the industry generally is cautious about technology readiness and the automotive market for carbon fiber. ORNL's carbon fiber systems integration and testing facility is a critical component in scaling the technology and demonstrating its readiness for commercialization. Significant further technology development, maturation, and scale-up is required before the new technology is ready for unsubsidized commercialization.

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Automotive Lightweighting Materials

Strain Rate Characterization of Advanced High Strength Steels

Background

In order to reduce weight and increase performance and safety of automobiles, U.S. automakers are increasingly using new grades of Advanced High-Strength Steels (AHSS). These new materials are used in structural components that are designed to withstand and manage high forces during crash and in-service conditions. New developments in metallurgy and processing of AHSS, together with advances in computer modeling, require accurate material characterization and verified models in order to take full advantage of the materials' higher strength.

Researchers at the Oak Ridge National Laboratory (ORNL) took on the task of developing and conducting material- and component-level experiments for the characterization of the crashworthiness of AHSS.

Technology

New experiments and computer models were developed to investigate the progressive crush in AHSS. The off-axis plate bending experiments (shown in Figure 2) replicate loading conditions that occur during the progressive crush of tubular-shaped structures and has a simple setup to minimize complexity of the test.

In addition, ORNL has developed structural component experiments using new, velocity-controlled, high-speed hydraulic equipment. Components are crushed in different modes to investigate crush efficiency and to characterize material responses.

Status

These new experiments are used to improve and verify

Figure 1. Different modes of progressive crushing lead to different amounts of energy dissipation in impact. Crushed in TMAC with 4 m/s.

Benefits

- New experiments are being developed for material crashworthiness characterization.
- Experiments are used for model validation and development of optimal designs.
- New methods and materials models will enable automotive designers to develop more efficient and safer designs more quickly.

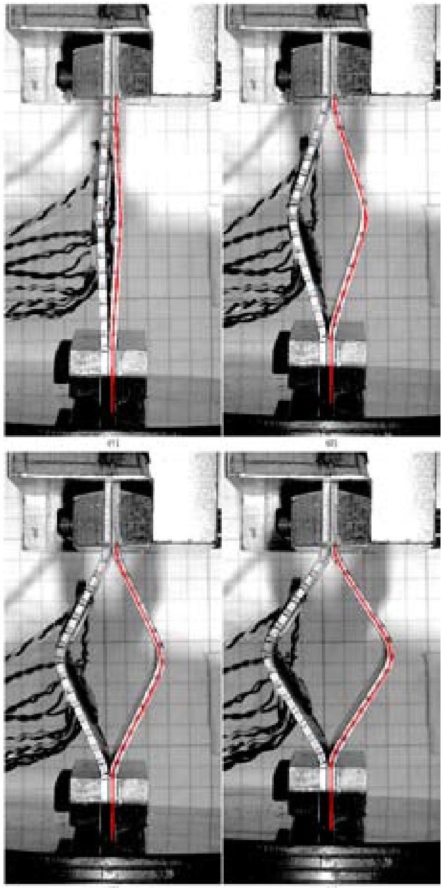

Figure 2. *Comparison of experiments and models (red) for double plate impact test.*

material models and computer modeling technologies for AHSS. Validated models will be distributed to steel manufacturers and automotive designers. New experimental setups and facilities are applied to new problems, such as modeling of strength of joints in impact, and further the advancement of crashworthy designs.

This particular effort has provided high-quality data for the development of material and structural computer models, enabling more accurate modeling and design of lightweight crashworthy vehicles.

Figure 3. *Test Machine for Automotive Crashworthiness (TMAC).*

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High Strength Weight Reduction Materials

Attachment Techniques for Heavy Truck Composite Chassis Members

Background

In terms of materials performance requirements, heavy vehicle chassis have components which are excellent candidates to potentially be replaced with low-density structural composite materials.

At the start of FY 2005, researchers at the Oak Ridge National Laboratory (ORNL) and the Pacific Northwest National Laboratory (PNNL) had already begun a research effort focused on developing joining techniques to overcome the technical issues associated with joining lightweight materials in heavy vehicles. The work is being performed concurrently with an industry program led by the National Composites Center to develop and commercialize composite chassis components, which will require resolution of the joining challenges. Different modeling techniques are being evaluated to assist in the performance prediction of potential joint designs.

Technology

Researchers at ORNL have been working closely with AlphaSTAR to build on the capabilities of its commercial software, GENOA, a progressive failure analysis tool developed specifically for fiber-reinforced composite materials. ORNL has worked with AlphaSTAR to develop and validate an interface between GENOA and the ABAQUS solver, which allows for contact modeling. This is critical for investigating damage in the composite at a bolted joint.

The resulting capability has been used to successfully evaluate the load distribution and damage in the composite due to bolt torque and subsequent loading of the bolted joint. Experimental testing validated the analytical results.

Commercialization

GENOA is commercially available software that has been used extensively in the aerospace industry to predict the strength,

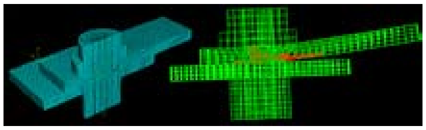

Figure 1. *GENOA model of bolted composite/steel joint with steel insert bonded to composite showing areas with damage.*

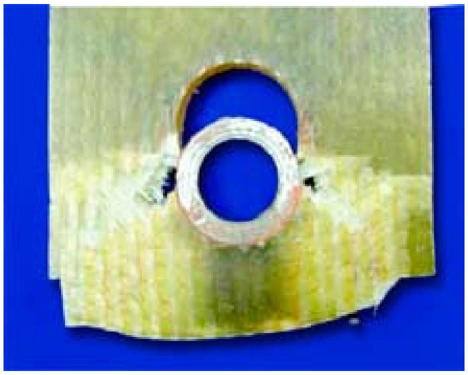

Figure 2. *Typical failure for a composite/steel lap shear specimen with a steel insert.*

Benefits

- The new software allows for more efficient design optimization of structural composite joints.
- The software will minimize required mechanical testing.

life and durability of composite components. This project is the software's first application to commercial vehicle design, specifically composite-to-metal structural joints. GENOA takes a full scale finite element model and breaks the material properties down to the microscopic level. The constituent properties are updated after each analysis iteration to reflect changes caused by damage or crack propagation.

ORNL and PNNL are working with AlphaSTAR to incorporate additional capabilities into GENOA software for optimization of bolted composite/steel joints for thick composite materials in a heavy vehicle chassis environment. The researchers are enhancing the software to make it more useful for the design of trucks and automobiles. The enhancements are being incorporated into new release versions of GENOA.

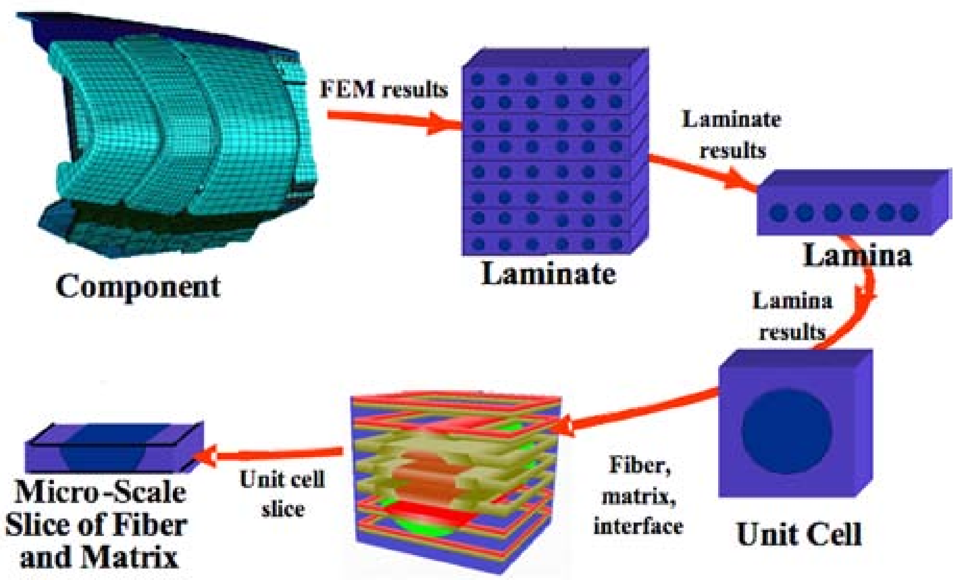

Figure 3. *Schematic of GENOA analytical hierarchy.*

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High Strength Weight Reduction Materials

Basic Studies of Ultrasonic Welding for Advanced Transportation Systems

Background

The transportation industry is aggressively pursuing high-performance, energy-efficient vehicles that involve the increased use of lightweight and high-strength materials [i.e., aluminum (Al) alloys, composites, magnesium (Mg) alloys, and advanced high-strength steels]. Using these new materials presents significant technical challenges to the existing body-assembly joining processes such as the electrical resistance spot welding (RSW). There are a number of issues in applying RSW to aluminum sheet metals and coated steels. Furthermore, due to the metallurgical incompatibility, fusion welding of dissimilar metals (e.g., aluminum to steel) is generally very difficult, if not impossible.

Researchers at the Oak Ridge National Laboratory (ORNL) are working on the ultrasonic welding process, a solid-state joining process. This process addresses the transportation industry's critical need for lightweight and high-performance materials in heavy-duty vehicles. Additionally, ORNL researchers are evaluating the feasibility of using the ultrasonic process as a low-temperature metal powder compaction process.

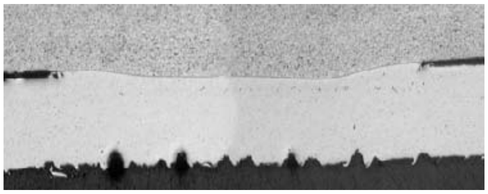

Figure 1. *UW bond between Al2024 and Al6061.*

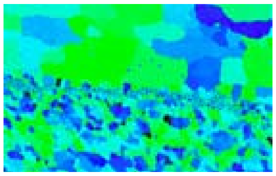

Figure 2. *Bonding interface microstructure.*

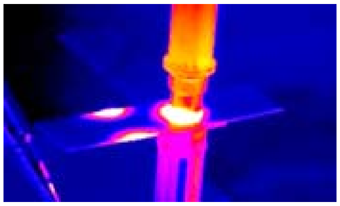

Figure 3. *Energy distribution during UW.*

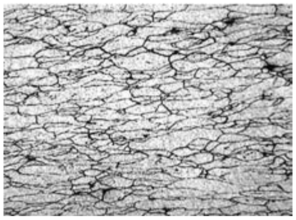

Figure 4. *Ultrasonic consolidation of Al powder.*

Technology

Ultrasonic welding (UW) uses high frequency mechanical vibrations to produce a solid-state metallurgical bond (weld) between metals. An electromechanical converter converts high-frequency electric current to mechanical vibrations. The mechanical vibration is typically at 20 to 40 kHz with an amplitude range of 5 to 50 mm. The power delivered to the

Benefits

- Provides a critical enabling joining process for increased use of high-performance lightweight material in heavy-duty vehicles.
- Offers high productivity due to its fast joining cycle and is extremely energy efficient due to its solid-state process nature.
- Enables low-temperature consolidation of materials produced by powder metallurgy.

workpiece ranges from several hundred to several thousand watts.

Thus far, Al, steel and Mg alloys have been successfully ultrasonic-welded. The feasibility of compaction and consolidation of metal powders has been demonstrated with Al powders. The joining of dissimilar metals (Al to Mg for example) is being investigated.

Status

Plans for continuation of this project include developing a clear understanding of acoustic wave propagation in the workpiece and its impact on weld quality, as well as developing an effective modeling capability to assist process optimization.

ORNL is pursuing opportunities for commercialization of this technology by identifying potential applications with its industry partners. ORNL plans to foster technology partnerships with other automobile/heavy truck manufacturers.

Figure 5. *Ultrasonic welding experimental apparatus.*

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High Strength Weight Reduction Materials

New ASTM Standard Test for Friction-Reducing Engine Materials

Background

Friction between moving parts robs engines of useful energy and lowers vehicle fuel economy. Depending on an engine's speed, the piston ring and liner system can account for over 50 percent of the total engine frictional losses. New materials, lubricants, and coatings can potentially reduce frictional losses; but the development cost for such materials can be high, especially when full-scale engine tests are involved. This project was initiated to develop a smaller-scale, cost-effective simulative laboratory test that correlated well with the material and lubricant performance in actual engines.

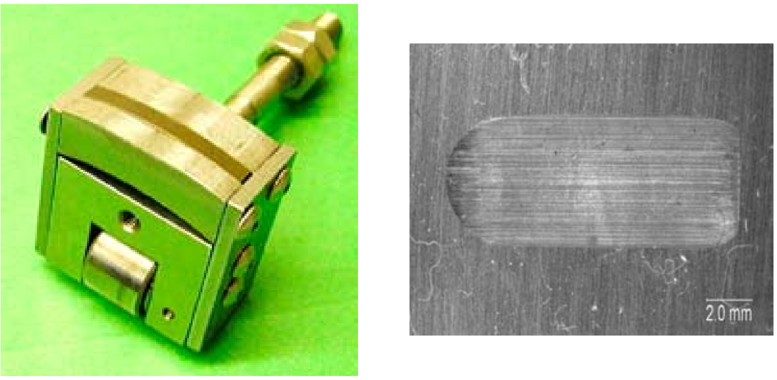

Figure 1. *(Left) The new test uses piston ring segments from production engines, held in place on specially-designed holders cut from diesel engine pistons. (Right) A typical wear mark from a 6-hour test on cast iron using high-soot diesel oil.*

Key elements required for effective ring/liner simulation were identified in FY 2001. In FY 2002, an industry advisory group was formed under the ASTM Committee G-2 on Wear and Erosion, and in FY 2003, friction and wear tests were conducted using new diesel and well-characterized, used diesel engine oils. In FY 2004, a draft standard practice was written and reviewed by the industry advisory group. After formal balloting, a new standard practice for friction

testing was approved by ASTM in early FY 2005 and designated as ASTM G-181-04.

Technology

A combination of mechanical, thermal, chemical and materials factors all interact to result in friction and wear behavior. Each of these variables was considered in developing the standard diesel engine ring and liner friction test. Because

Benefits

- Provides ability to screen promising new materials and surface treatments for possible piston ring and liner use.
- Simulates the effects of realistic engine oils on friction, accounting for effects like exhaust gas recirculation, oil acidity, and soot build-up.

engine designs differ, the standard was developed so testing parameters could be adjusted to simulate a range of engines and lubricant characteristics.

A set of well-characterized, standard test oils from Southwest Research Institute was used to verify the ability of the new test method to detect effects of oil condition on the friction of new, lightweight engine materials.

Commercialization

The new ASTM standard practice for friction testing is now ready to assist diesel engine designers and manufacturers in selecting new materials and surface treatments for piston rings and liners. The Oak Ridge National Laboratory (ORNL) will include the new procedure within the suite of friction and wear research capabilities offered to industry for collaborative research under the High Temperature Materials Laboratory User Program.

A companion ASTM standard for wear testing of piston rings and cylinder liners is also under development under ORNL leadership. It will soon provide the ability to cost-effectively

Designation: G 181 – 04

Standard Practice for
Conducting Friction Tests of Piston Ring and Cylinder Liner Materials Under Lubricated Conditions[1]

This standard is issued under the fixed designation G 181; the number immediately following the designation indicates the year of original adoption or, in the case of revision, the year of last revision. A number in parentheses indicates the year of last reapproval. A superscript epsilon (ε) indicates an editorial change since the last revision or reapproval.

1. Scope

1.1 This practice covers procedures for conducting laboratory bench-scale friction tests of materials, coatings, and surface treatments intended for use in piston rings and cylinder liners in diesel or spark-ignition engines. The goal of this procedure is to provide a means for preliminary, cost-effective screening or evaluation of candidate ring and liner materials. A

3. Terminology

3.1 *Definitions of Terms Specific to This Standard:*

3.1.1 *conditioned oil*—a lubricating oil whose viscosity, composition, and other function-related characteristics have been altered by use in an operating engine, such that the oil's effects on friction and wear reflect those characteristic of the long-term, steady-state engine operation.

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Automotive Propulsion Materials

Effect of Thermal Cycling on the Properties of NdFeB Permanent Magnets

Background

New technologies, such as permanent magnets for motors, sensors, and control systems, are necessary for achieving FreedomCAR and Vehicle Technologies Program goals. Such magnets will have to operate reliably over a wide range of temperatures and be resistant to thermal cycling.

To support those developmental efforts, ORNL built an experimental test facility to assess the effect of temperature and thermal cycling on the magnetic and mechanical properties of permanent magnets.

Technology

The experimental test facility developed at ORNL consists of an environmental chamber capable of operating between -100°C and 300°C. Test temperatures below ambient temperature are attained by dispersing liquid nitrogen using compressed air, while higher temperatures can be attained by using compressed air and cartridge heaters. The interior of the 61 × 30 × 30 cm^3 chamber is lined with insulation to ensure uniform temperature distribution.

A computer-based system was assembled for data acquisition and control. This system includes a personal computer, a high-speed A/D data acquisition card, customized software written with LabView® and a digital temperature controller. Inside the environmental chamber an array of sixteen 6.5-mm diameter rods is mounted onto a frame that is connected to a pneumatic actuator. The permanent magnets under evaluation, which are shaped in the form of prismatic beams, are mounted using a removable adhesive at various locations along the rods. A series of coils, which are concentric to the rods, were placed at fixed locations.

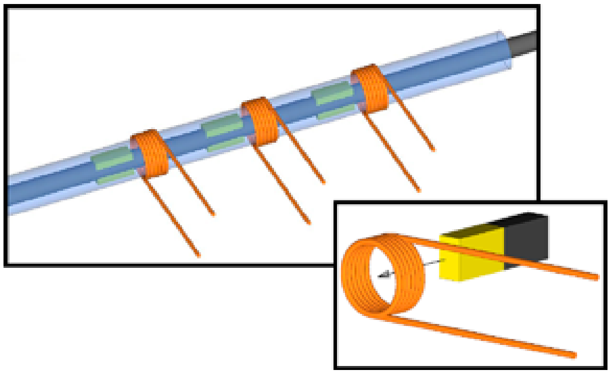

Figure 1. *Faraday's law is used to determine the magnetic strength of permanent magnets.*

Benefits

- A test facility was developed to help designers of automotive components that incorporate permanent magnets to determine how the properties of magnets change as a function of temperature and thermal cycling.
- This facility is available to industry and academic institutions as part of the High Temperature Materials User Program.

When the pneumatic actuator is activated, the rods, and the magnets, slide through the coils, inducing in turn a voltage across the terminals of the coils. According to Faraday's law the voltage induced in the coil is proportional to the change in the magnetic flux through the coil, according to:

$$V = -\frac{d\Phi}{dt} = -\,N\,A\,\frac{dB}{dt}$$

where B(t) is the magnetic field of the magnet, N is the number of turns in the coil, and A is the crosssectional area of the coil.

The voltage induced is recorded as a function of temperature and the number of thermal cycles. Therefore, by measuring the voltage it is possible to determine if any changes have occurred in the magnetic strength of the magnet under evaluation.

After a predetermined number of thermal cycles, test specimens are removed from the environmental chamber and evaluated in a fourpoint bending to assess the effect of thermal cycling on their mechanical strength.

Status

It has been found that the magnetic strength of bonded and sintered permanent NdFeB magnets decreases linearly with temperature and that at a given temperature, it decreases exponentially with the number of thermal cycles.

It was also found that sintered NdFeB magnets were 10 times stronger than bonded NdFeB magnets and that the flexural strength of both decreased with the number of thermal cycles.

Figure 2. *Experimental test facility to evaluate the thermal cycling resistance of permanent magnets.*

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Heavy Vehicle Propulsion Materials

Thermal Oxidation: A Promising Surface Treatment for Titanium Engine Parts

Background

Recent advances in lower-cost titanium (Ti) processing, coupled with its potential use as a lightweight material in heavy-duty diesel engines and brakes, has prompted interest in friction and wear-related applications for Ti alloys.

Originally developed for aerospace use, Ti alloys offer an excellent combination of mechanical properties and corrosion resistance; however without protection, they tend to gall when rubbed against other metals. Attempts to lubricate Ti met with limited success. Tests at the Oak Ridge National Laboratory (ORNL) have shown that conventional 15W40 diesel engine oil does not effectively lubricate Ti-6Al-4V, the most popular Ti alloy. While Ti-6Al-4V is stronger and harder than gray cast iron, it exhibited three times the friction coefficient and wore 2,000 times faster than cast iron, when tested against production grade Cr-plated diesel engine piston rings. Thus, Ti alloys are good candidates for advanced surface engineering.

Material	Non-treated Ti_6Al_4V	Thermally Oxidized Ti_6Al_4V	Improvement
Hardness (HK, GPa)	3.3	22.7	7 Times Harder!
Friction Coefficient	0.37	0.11	70% Lower!
Wear Rate (mm^3/N-m)	3.7×10^{-4}	5.9×10^{-9}	60,000 Times Lower!

Figure 1. *Friction and wear results for non-treated and thermally-oxidized Ti6Al4V alloy against a Cr-plated ring in 15W40 diesel oil.*

Processing and cost limitations of sophisticated surface treatments and coating methods limit their use on titanium alloys in certain friction and wear applications.

Technology

Thermal oxidation (TO) offers the potential to significantly improve the wear resistance of Ti alloys while also reducing friction. Heat treating a Ti alloy to several hundred degrees Celsius in either air or a binary gas mixture, produces a micrometer-thick TiO_2 surface layer and an underlying oxygen-enriched layer. The TO process is relatively simple to apply,

Benefits

- Thermal oxidation dramatically lowers the friction and wear of Ti alloy surfaces.
- Thermal oxidation is relatively simple to apply, low cost, and not restricted by part shape or size.
- Thermal oxidation enables certain lubricant additives which were designed for iron-based alloys to work on titanium alloys as well.

is inexpensive, and is not so restricted to simple shapes as are many other coating methods.

Recent friction and wear tests in diesel oil, conducted at ORNL, revealed impressive benefits of TO. As Figure 1 indicates, when compared with bare Ti-6Al-4V, the friction coefficient of the treated alloy was reduced by more than three times, and the wear rate was even more impressively reduced.

Ti-6Al-4V specimens were thermally oxidized, then tested using ASTM G 181-04, a new standard practice for diesel engine piston ring and liner friction testing that was recently developed at ORNL under DOE sponsorship.

The TO surface was much harder, had lower friction coefficient and astonishingly low wear compared with the bare alloy. Figure 2 shows a marked decrease in wear damage from using TO.

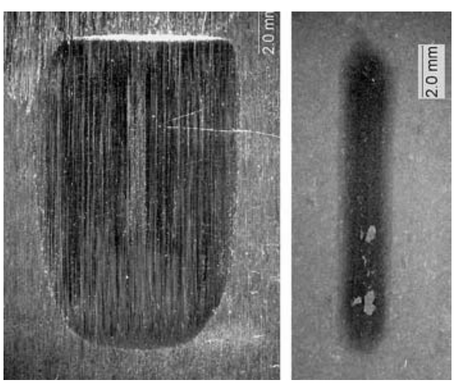

Figure 2. *Wear scars on non-treated (left) and thermally-oxidized (right) Ti6Al4V.*

Compared to conventional cast iron, the TO-treated Ti-6Al-4V had comparable friction, but 1,000 times less wear. These results far exceed expectations based on the research published by others. Remarkably, the oxygen diffusion layer beneath the titanium dioxide crust has good friction and wear behavior even after the crust was worn through. That observation flies against assumptions that failure of the oxide layer marks the end of useful life.

Surface chemical analyses are beginning to elucidate the basic science of how TO works on titanium alloys. This research is a promising new advance toward light-weight, corrosion-resistant engines of the future.

Status

As simple and cost-effective as it is, thermal oxidation has a great untapped potential to expand the use of Ti alloys for wear- and friction-critical bearing surfaces, like heavy-duty diesel engines. Future commercialization options are being explored.

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Heavy Vehicle Propulsion Materials

Development of Materials Analysis Tools for Studying NO_x Adsorber Catalysts

Background

In order to meet the 2007 emission requirements for diesel exhaust, engine aftertreatment will be needed. The necessary technology will need to integrate aftertreatment with engine control systems. Currently, no commercial off-the-shelf technologies are available to meet the 2007 standards. Consequently, Cummins, Inc., is working to understand the basic science necessary to effectively utilize these catalyst systems. The Oak Ridge National Laboratory (ORNL) is assisting Cummins with the materials characterization effort.

Technology

Base-metal oxides (BMOs) are major components in current NO_x adsorber catalysts which Cummins seeks to use in aftertreatment systems. Although the function of these adsorbers is to collect surface nitrite/nitrate (NO_x) species, they also collect oxy-sulfur (SO_x) species. Both species are to be released from these surface sites during different regenerations, where the adsorber BMO is either heated to some critical temperature and/or exposed to a reducing or reactant atmosphere. Sulfur adsorption is unfortunately a form of poisoning to adsorber catalysts. It is a major problem that must be resolved before BMO-based emission reduction technologies become commercially viable.

Status

The crystal structure, morphology, phase distribution, particle size and surface species of catalytically active materials supplied by Cummins will be characterized using X-ray diffraction (XRD), Raman spectroscopy, and electron microscopy. These materials will come from all stages of the catalyst's life cycle: raw materials, as-calcined, sulfated, regenerated, etc.

Pt is the catalytically active element which must remain dispersed and of small size within the adsorber. Past work has shown Pt particle growth

Figure 1. *A Cummins ISX engine.*

Benefits

- Addresses a major technical barrier to long-term viability of NO_x adsorber catalyst.
- Assists heavy-duty diesel engines in meeting 2007 requirements for NO_x emissions.

as a function of desulfation time in lab-based engine tested samples. Last year, evaluation of gradient formation of active elements on a macro scale was investigated on catalysts.

A scanning transmission electron microscope (STEM) was employed to examine the gradient of Pt particle size along the length of a catalyst sample taken from a cordierite "brick." Figure 2 shows the Pt particle sizes to be the same at both ends of the sample. The bright spots in the STEM images are the Pt particles. Multivariate statistical analysis, an analysis procedure for spectral image datasets, was applied to extract the particle size distribution from 10 images of each section. While the distributions appear to be different, the average and median sizes are effectively the same. The XRD results also showed negligible particle/crystallite size change along the length of the sample, but did not agree with respect to size. Superposition of the Pt and washcoat peaks will require synchrotron XRD to resolve.

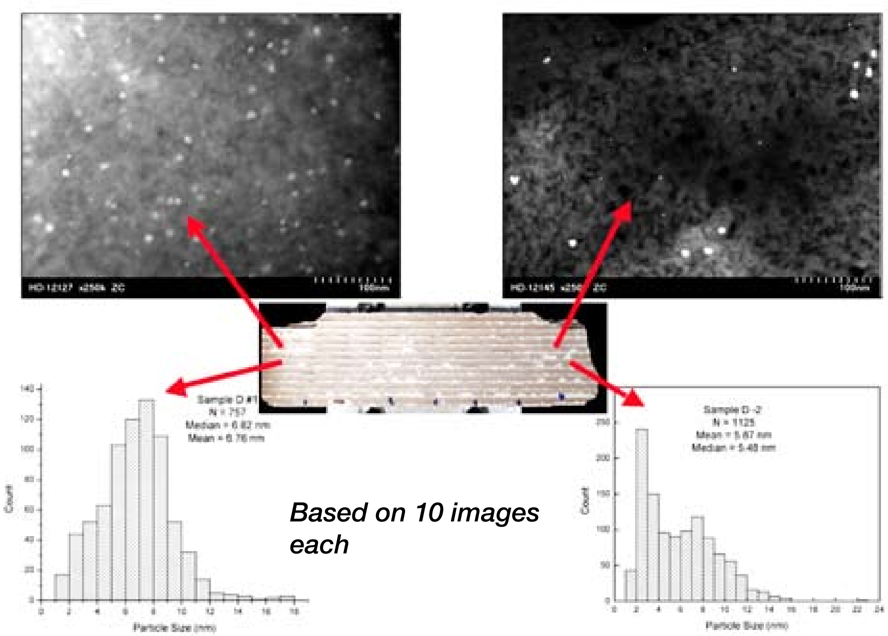

Figure 2. *HA-ADF image from the STEM showing Pt particles in bright contrast and the corresponding size distributions.*

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Heavy Vehicle Propulsion Materials

NO_x Sensors for Heavy Vehicles

Background

Environmental concerns are driving efforts to reduce pollutant emissions from mobile power sources. Nitrogen oxides (NO_x) are one of the pollutants of primary concern. Unfortunately, no catalyst presently exists that can decompose NO_x in the O_2-rich exhausts from diesel and lean-burn gasoline engines. Thus techniques such as the lean NO_x trap (LNT) and selective catalytic reduction 8(SCR) are being explored for NO_x remediation. On-board NO_x sensors are required for either approach, to control trap regeneration (LNT) or reagent injection (SCR). A suitable sensor would demonstrate the following characteristics:

- operate at temperatures around 600–700°C;
- measure NOx in the range 1 ppm $\leq$ [NOx] $\leq$ 1000 ppm;
- exhibit no cross sensitivity; and
- response time of less than 1 second.

Technology

Above room temperature, NO_x primarily consists of NO and NO_2. Because equilibrium conditions can not be assumed to prevail in the exhaust, it may be necessary to measure two of the these three concentrations in the exhaust; [NO], [NO_2], and [NO] + [NO_2].

The last of these, ([NO] + [NO_2]), is often called "total NO_x." At ORNL, scientists are developing sensors that can measure "total NO_x" and sensors that can selectively measure [NO]. The sensors under development are based on yttria-stabilized zirconia (YSZ), a material that is already widely used in O_2 sensors for combustion exhausts. Electrodes are applied by screen-printing and thermal treatment, techniques that are widely used today in the hybrid circuit manufacturing industry.

Status

This effort is still ongoing and

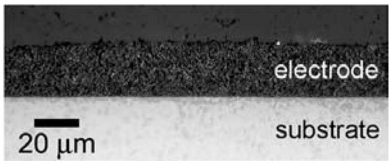

Figure 1. Cross-section shows electrode thickness.

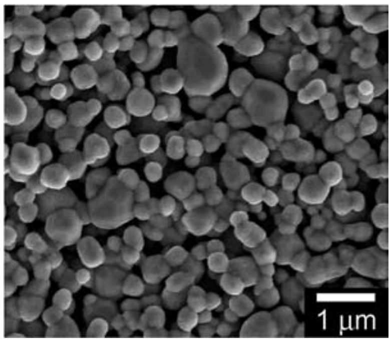

Figure 2. Electrode microstructure is designed to be porous.

Benefits

- Allows measurement of NO from 1 to 1000 ppm.
- 90% response/recovery times at ≈1 sec.
- No CO, SO_2, and HC cross sensitivity.
- Inexpensive manufacturing process.

extensive testing is under way to understand and eliminate cross sensitivities. This project is a CRADA with Ford Motor Company and is being performed in collaboration with Lawrence Livermore National Laboratory. The interaction of such a multidisciplinary team will provide a clear path to commercialization.

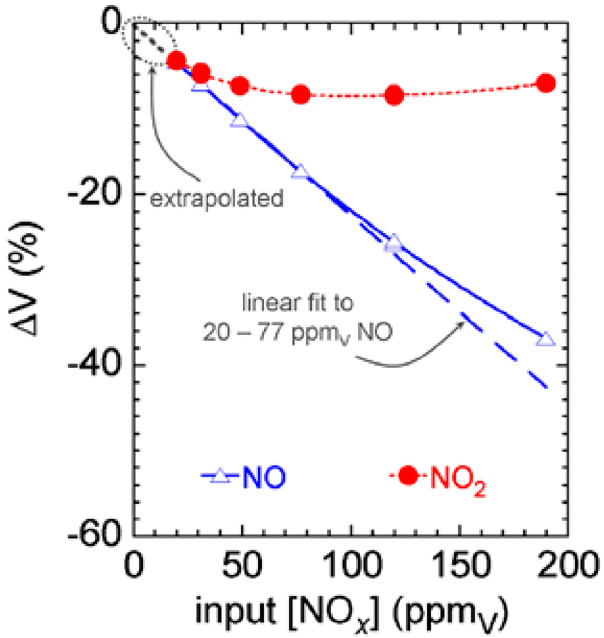

Figure 3. *"NO-selective" sensing behavior at 600 °C and 7 vol % O_2.*

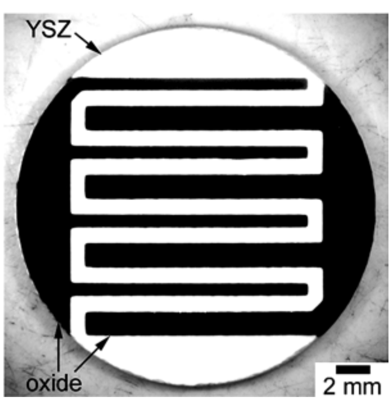

Figure 4. *Prototype sensing element on YSZ substrate.*

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Heavy Vehicle Propulsion Materials

Durability and Reliability of Porous Cordierite Diesel Particulate Filters

Background

Diesel engines are the most efficient internal combustion engines today. However, concerns with diesel emissions (nitrogen oxides and particulate matter) have prompted stringent environmental regulations that will become effective in 2007 and 2010. Diesel particulate filters (DPFs) are one of the leading technologies to address these regulations. A DPF is a device that collects particulate matter in the exhaust stream. The high temperature of the exhaust heats the structure and allows the particles inside to break down (or oxidize) into less harmful components. DPFs can reduce emissions of particulate matter, hydrocarbons and carbon monoxide by 60 to 90 percent.

Most DPFs consist of a ceramic honeycomb with hundreds of cell passages partitioned by walls. Each cell passage has a square cell opening at one end and is closed at the other end so that the cell passages are alternately closed at each end. This structure forces the exhaust gases through the porous, thin ceramic honeycomb walls. When the gases carrying the particulates flow through the fine pores of the walls, the particulates are filtered out of the exhaust gases.

High porosity values help attain filtration efficiency greater than 90 percent while reducing gas-flow resistance to prevent affecting engine performance.

Technology

Cummins, Inc., is working with Oak Ridge National Laboratory (ORNL) to develop models to predict the durability and reliability of DPFs. The formulation of such models requires knowledge of the distribution of temperatures and stresses to which DPFs will be subjected during service in addition to how these factors and the service environment affect the thermophysical properties of DPFs as a function of time. This is a challenging goal because DPFs are expected to operate for more than 400,000 miles and to experience possibly thousands of regeneration cycles.

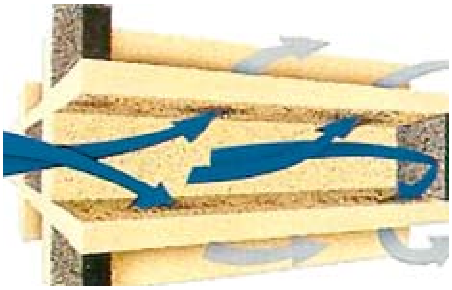

Figure 1. Cordierite diesel particulate filters.

Benefits

- Provides property data needed to predict durability of a leading DPF candidate material.
- Helps diesel engines to meet 2007 and 2010 emissions regulations with no fuel penalty.

Fracture toughness and resistance to environmentally assisted crack growth are two key properties that need to be known to predict the reliability and durability of DPFs.

In this project test methods have been developed to determine these properties for porous cordierite, which is one of the leading candidate materials for the manufacture of DPFs.

Test specimens 280-μm thick were prepared, notched, pre-cracked and evaluated by the double-torsion test method to determine fracture toughness. This same test method was used to determine the resistance of porous cordierite to environmentally assisted crack growth at elevated temperatures. The fracture toughness of porous cordierite was found to decrease with temperature from 0.45±0.02 MPa√m at 20°C to 0.36±0.07 MPa√m at 500°C. It was also found that the crack trajectory was significantly influenced by the microstructure of the material, in particular the morphology of pores and their distribution.

Status

Scientists and engineers at ORNL and Cummins are collaborating to develop models to predict the reliability and durability of porous cordierite diesel particulate filters. They are also developing filter regeneration and control strategies that will help meet environmental regulations while preserving the fuel efficiency of future diesel engines

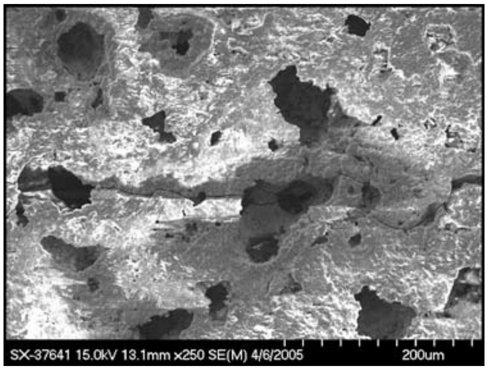

Figure 2. Scanning electron micrograph illustrating the interaction between the microstructure of porous cordierite and the propagation of cracks.

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Heavy Vehicle Propulsion Materials

Catalysts by First Principles

Background

The high loading of precious metals to overcome gradual and persistent deterioration of the performance of three-way catalysts for after-treatment of engine out emissions is rather well-known. This deterioration has been found to be rapid in supported catalyst systems that operate under oxidizing environment (e.g., lean NO_x traps, oxidation catalysts, HC-SCR, etc.). However, alleviating performance deterioration through the traditional catalyst development approach has not been successful in this instance.

Despite dramatic improvements in experimental and theoretical bases for their characterization, the traditional approach to catalyst development is still dominated by trial and error methods. Although it has been successful, the empirical development of catalytic materials is time consuming and expensive and brings no guarantees of success. In addition, experimental catalysis has not benefited from the advances in high performance computing that enables more realistic simulations (empirical and first-principles) of large ensemble atoms including the local environment of a catalyst site in heterogeneous catalysis.

Thus, a protocol to systematically find the optimum catalyst can be developed that combines the power of theory and experiment in an iterative process for atomistic design of catalytically active sites and can directly translate the fundamental insights gained to a complete catalyst system that can be technically deployed (shown in Figure 1).

Technology

The theoretical modeling is based on DFT studies of Pt clusters to understand the relationship between cluster size, structure, composition, and reactivity. This, coupled with first-principles thermodynamics, provides insights into the effects of oxidizing atmosphere (O_2) – finite (T, pO_2), structure, composition, redox potential on

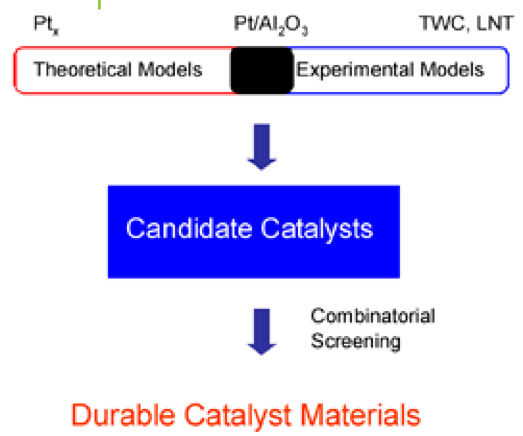

Figure 1. *A protocol that combines the power of theory and experiment in an iterative process to systematically find optimum catalysts.*

Benefits

- Enables faster, less expensive catalyst development.
- Determination of reactive catalyst site structure enables design of durable catalysts with optimal operation.

particle size. The results provide guidance for investigations of larger/supported clusters. Experimentally, researchers have synthesized a series of Pt and Re clusters and particles supported on morphologically different γ–aluminas. The microstructural characterization reveals structural differences in 1-3 atom and 10-20 atom clusters.

Theoretical models reveal that Pt nanocluster reactivity shows strong size dependence. Small clusters are much more prone to oxidation and oxidized clusters adopt 1-D or 2-D structures. Higher temperature or lower pO_2 leads to less oxidation and lower oxide phases are more prevalent for larger clusters. Increasing temperature leads to increased oxidation of Pt oxide clusters but reduction of clusters becomes more facile.

Experimentally, researchers have synthesized a variety of stabilizer incorporated aluminas with controlled surface properties (e.g., sol-gel, mesoporous molecular sieves etc.) that are stable to thermal treatment (~900°C). The synthesis and characterization of carbonylated, decarbonylated, and nanoclusters of precious metals (Pt, Re) on these aluminas have also been completed. Figure 2 shows 10-20 atom Pt nanoclusters on γ-alumina. This structure is an input for theoretical modeling of Pt/γ-alumina materials.

Status

The reactivity of precious metals

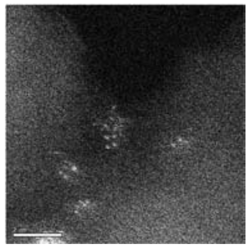

Figure 2. *HA-ADF image from the STEM showing Pt particles.*

(carbonylated, decarbonylated, and nanoclusters) on γ-alumina (commercial, sol-gel, and mesoporous molecular sieve) are currently being examined for the oxidation of CO, HC, and NO_x to determine the structure of reactive catalyst sites. This iterative process will lead to the identification of optimal catalyst sites for CO, HC, and NO_x oxidation. These results will enable the design of durable catalysts containing such sites for optimal operation.

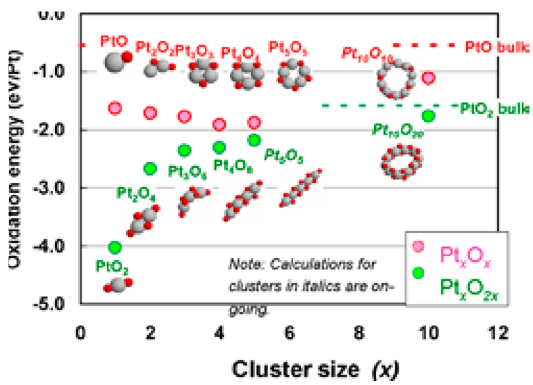

Figure 3. *Oxidation energies of the Pt_XO_X and Pt_XO_{2X} clusters.*

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Heavy Vehicle Propulsion Materials

Ultra-high Resolution Electron Microscopy for Catalyst Characterization

Background

The new aberration-corrected electron microscope (ACEM) is now in its first year of full beneficial operation. It has been employed in several studies to better understand the structures of catalyst materials for reduction of emissions of nitrous oxides in automotive and diesel exhaust systems. The ACEM is the first such microscope in the nation that is located in a user facility. It supports not only Energy Efficiency and Renewable Energy (EERE) Program catalyst studies, but also a variety of user projects that are related and that provide synergistic information to aid in the understanding of catalyst micro-structure, behavior, and poisoning mechanisms. Utilizing the "annular dark-field" or so-call "Z-contrast" imaging mode, the instrument provides sub-Ångström (1 Å = 0.1 nm) images that show high atomic number atomic species in bright contrast, directly related to relative atomic number. Thus, it is now possible to image single atoms, ultra-fine clusters, and "rafts" of atoms that are precursor structures in typical as-prepared catalyst systems.

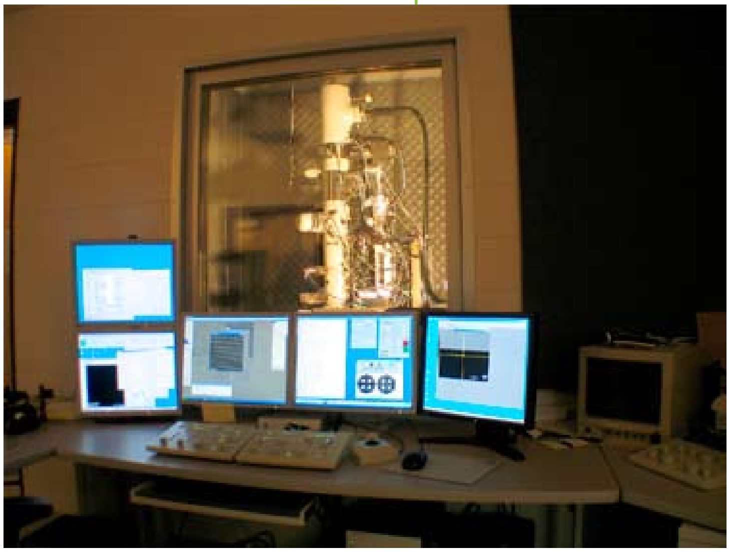

Figure 1. *JEOL 2200FS-AC aberration-corrected STEM/TEM, seen through a window in the control room. All alignments and other operations are controlled using an associated knobset, and mouse clicks within the digital imaging software.*

The goal of this research is to find effective methods to control the morphology of the catalytic during use so that optimum performance can be maintained. Outstanding results have been obtained recently in studies of rhenium and platinum catalysts on alumina support materials.

Benefits

- The most advanced catalyst imaging capability made available to DOE programs.
- Will further the understanding of the important mechanisms for catalyst deactivation with use.

Technology

To assure that the ACEM can achieve its optimum resolution on a routine basis, the instrument is housed in the new Advanced Microscopy Laboratory, located at the Oak Ridge National Laboratory (ORNL). This new facility was designed to provide an environmentally 'quiet' environment for ultra-sensitive instruments. The ACEM is operated remotely, from an adjacent control room, as shown in Figure 1. This capability also allows it to be accessed from any other remote location, which will greatly facilitate collaborative research with outside partners.

The ability of the ACEM to characterize catalyst microstructures at the atomic level is shown most spectacularly with the imaging of rhenium (Rh) clusters on γ-alumina. In this work with Prof. Bruce Gates of the University of California, Davis, Rh-carbonyl clusters containing only 3 Rh atoms were distributed on the surfaces of fine alumina support particles. The clusters cannot be detected in a bright-field image due to the high phase contrast of the support structure. In dark-field mode, however, the strongly scattered electron intensity from the Rh reveals the species in bright contrast. Figure 2 shows single atoms (A), a 3-atom trimer (B), and an apparent dimer (C). As indicated in Figure 3, the dimer shows double the intensity of one atom versus the other,

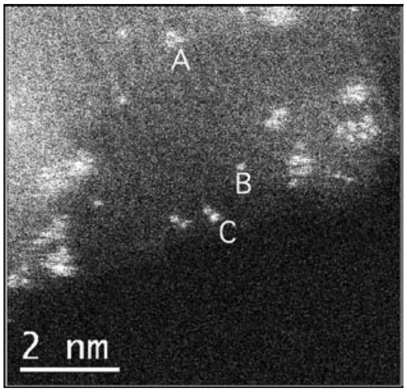

Figure 2. *Dark-field mode reveals rhenium clusters on alumina.*

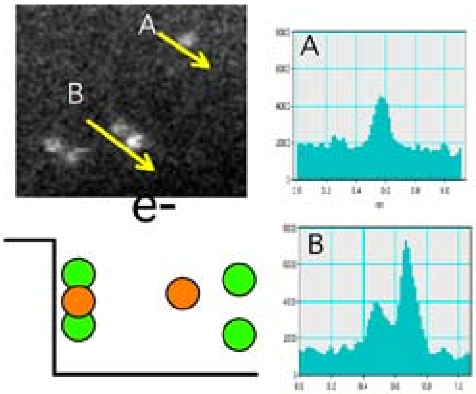

Figure 3. *Enlargement of apparent rhenium dimer reveals significant difference in intensity of atoms.*

suggesting that we are imaging a trimer edge-on, perhaps tethered to a ledge on the alumina surface, as indicated by the cartoon.

Status

This is the first time such a capability for catalyst characterization at the atomic level has been unambiguously demonstrated. This capability will be further utilized in advanced studies of catalysts of interest in the FCVT Program.

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A Strong Energy Portfolio for a Strong America

Energy efficiency and clean, renewable energy will mean a stronger economy, a cleaner environment, and greater energy independence for America. Working with a wide array of state, community, industry, and university partners, the U.S. Department of Energy's Office of Energy Efficiency and Renewable Energy invests in a diverse portfolio of energy technologies.

Heavy Vehicle Propulsion Materials

Microstructure-based FEA (μ-FEA)

Background

Microstructure-based FEA (μ-FEA) is a copyrighted, Oak Ridge National Laboratory (ORNL)-developed, LabView-executable program that enables stress analysis of real and simulated material microstructures via direct integration with ANSYS finite element analysis (FEA) software.

μ-FEA enables the user to capture the complexity of actual microstructures through simple and automated input of digital images taken with a SEM or optical microscope.

μ-FEA enables the user to readily examine and interpret resulting stresses in microstructures or compare stresses through simple changes in boundary or initial conditions or architectures. “What-if?” analysis is easily performed.

Because ANSYS is used as the FEA Solver, the full multi-physics suite of ANSYS features is exploitable (e.g., linear and nonlinear properties, steady-state and transient analysis, piezoelectric effects, phase changes and swelling, sensitivity and probabilistic analysis, etc.).

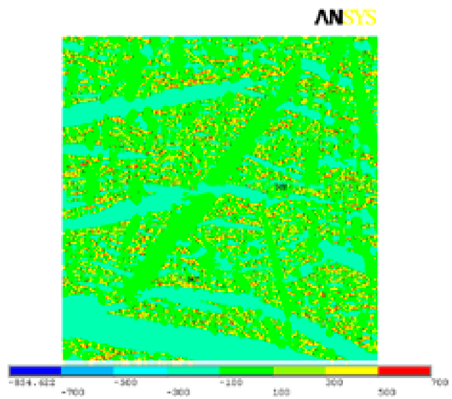

Figure 1. *Thermoelastic residual stresses in an Si_3N_4 microstructure.*

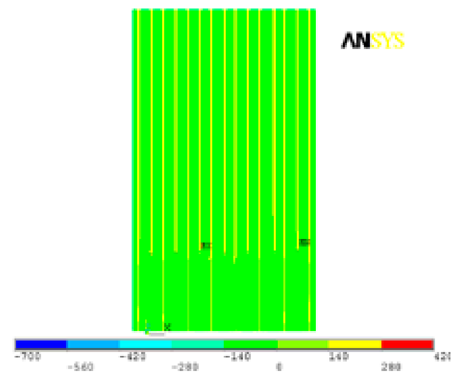

Figure 2. *Thermoelastic residual stresses at the margin in a PZT piezostack.*

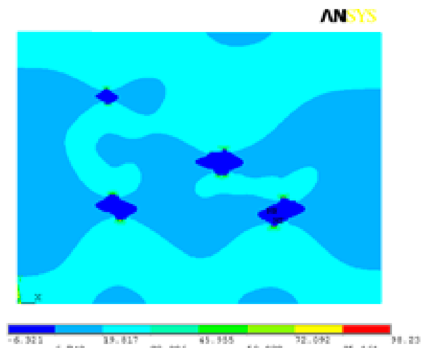

Figure 3. *Stresses about microstructural pores in a poled PZT piezoceramic*

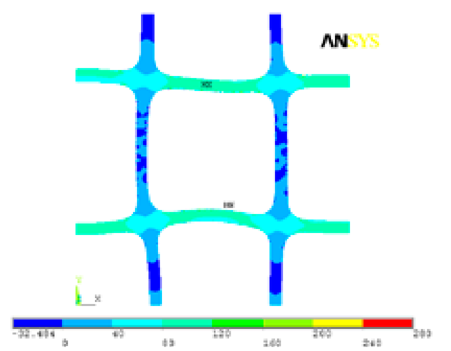

Figure 4. *Residual stresses about a diesel particulate filter unit cell.*

If the user can take a picture of a microstructure, then μ-FEA can be used to help analyze it.

Benefits

- Microstructural engineering.
- Device design optimization.
- “What-if?” design refinements.
- Virtual characterization.

Technology

μ-FEA is currently used to explore stress fields and for microstructural engineering in material systems and devices relevant to a variety of transportation-related applications:

- Tribological coatings
- Thermal barrier coatings
- Piezoelectric devices
- Thermoelectrics
- Advanced silicon nitrides
- Diesel particulate filters
- Graded microstructures resistant to contact damage

Commercialization

μ-FEA software was copyrighted in June 2005.

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A Strong Energy Portfolio for a Strong America

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Heavy Vehicle Propulsion Materials

Microstructural Changes in NO_x Trap Materials Under Lean and Rich Conditions at High Temperatures

Background

The introduction of diesel engine-based, heavy-duty trucks and passenger vehicles depends upon the successful development of a strategy to treat nitrogen oxide (NO_x) emissions. A catalyst or combination of catalysts that can convert NO_x into inert gases under oxidizing conditions over a complete range of exhaust temperatures does not presently exist. Among NO_x treatment strategies, lean traps (LNT) are the most likely candidates for early deployment because they are consumer transparent (no action needed on the part of consumers), and they can be system-integrated into current vehicle control strategies.

The basic components of NO_x traps are identical to three-way catalysts. The NO_x traps derived from advanced three-way catalysts are two-layer systems on a honeycomb substrate with the inner layer based on platinum-alumina and the outer layer on rhodium-ceria-zirconia. In addition, there is high baria content (the upper limit being close to 20 percent) in the alumina layer. Fresh NO_x traps work very well but cannot sustain their high efficiency over the lifetime of vehicles.

The performance deterioration in NO_x traps is believed to be caused by aging due to high-temperature operation and sulfation-desulfation cycles necessitated by the sulfur oxides in the emissions from the oxidation of sulfur in fuel.

Technology

Studies of the microstructural changes that occurred in a supplier lean NO_x trap system (two layers: Pt/BaO-Al_2O_3 and CeO_2-ZrO_2) upon aging on 1) a pulsator at Ford, 2) dyno at Ford, and 3) on vehicles in gasoline DISI engines in Europe, show that the sintering and migration of precious metals and migration of barium leads to reduced precious metal-adsorber surface area available for NO_x adsorption in lean cycles.

Figure 1. *Ex-situ reactor allows rapid screening of catalysts for microstructural changes under simulated operating conditions and accelerated aging conditions.*

Benefits

- Better understanding of catalyst response to thermal cycling for desulfation.
- Correlation of microstructure changes with catalyst performance facilitates rapid development of durable, effective catalysts.

In order to design a thermally durable NO_x trap, there is a need to understand the changes in the microstructure of materials that occur during various modes of operation (lean, rich, and lean-rich cycles). Oak Ridge National Laboratory (ORNL) scientists have designed an ex-situ reactor system that allows for the rapid screening of microstructural changes in catalyst materials upon extended exposure to operating conditions or accelerated aging conditions suing simulated exhaust (see Figure 1).

For rapid screening, the catalyst samples are deposited on specially designed transmission electron microscopy grids. The sample grid is then transferred to a TEM and several areas of sample are imaged. The grid is then placed in the ex-situ reactor and exposed to lean, rich, or lean-rich cycle using a simulated exhaust gas stream. The samples are transferred to TEM and the original areas are examined again. This approach allows us to accurately monitor microstructural changes in a sample and eliminates averaging effects common to several other techniques (e.g., spectroscopic methods, XRD, EXAFS, XANES etc.).

For example, the accelerated aging of model catalyst, 2% Pt-98% [10% CeO_2-ZrO_2-90% (2% La_2O_3-98% $BaO \bullet 6Al_2O_3$)], was carried out using simulated exhaust under a lean-rich cycle. Interestingly, Pt sintering was evident after only 4 hours of sample treatment under accelerated aging conditions. A gradual growth in Pt particles in the 2.0-5.0 nm range was seen after each additional four hours of treatment.

Status

The efforts to correlate the microstructural changes with catalyst performance are in progress. The results will allow us to rapidly screen samples for microstructural changes and thereby for performance facilitating rapid development of durable catalysts.

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Vehicle Systems

Heavy Vehicle Duty Cycle

Figure 1. Dana tractor/trailer being fitted with sensors and data acquisition system.

Background

The U.S. trucking industry involves considerable use of class 8 trucks and operates in relatively small fleets; 50% of the fleets in the U.S. comprise less than 100 trucks and 25% are less than 10 trucks). The industry operates on a small profit margin and is faced with regulatory and economic pressures. Making heavy trucks more efficient through new technologies and fleet management protocols would reduce dependence on oil and release of emissions into the environment, as well as contribute to larger profit margins. Since efficient systems are typically inherently safer, lives could also be saved.

One obstacle involves knowing what the true benefits are of new energy efficient technologies. Most benefit assessments are based on existing information on heavy truck operation. Much of this information is stylized and based on duty cycles that are meant to test various emission or fuel economy measurements. For example, the FTP Transient Cycle is a transient engine dynamometer cycle for heavy-duty truck and bus engines. It includes segments designed to simulate both urban and freeway driving and used for emission certification testing of heavy-duty diesel engines in the United States. Another example is the Urban Dynamometer Driving Schedule (UDDS), which is an EPA transient chassis dynamometer test cycle for heavy-duty vehicles. While cycles such as these are based on an understanding of the vehicle technologies and how the best vehicles might be tested to assess emissions and fuel economy, they do not accurately reflect real world driving.

Benefits

- Supports the development and calibration of Argonne National Laboratory's PSAT Class 8 module.
- Supports the development of a tool to generate customized duty-cycles for input to simulation models and other applications.
- Enables better-informed technology investment decisions.

How trucks actually operate on highways is not well understood. Only an experienced heavy truck driver has a true situational awareness of the characteristics of driving on our nation's highways. There are many factors that affect operations, such as

- rules on hours of operation,
- recurring congestion in urban envrionments,
- non-recurring congestion (road construction or accidents, for example),
- anti-idling regulations,
- differing fleet management philosophies,
- weather, and
- topological conditions.

A better understanding of the effects these and other factors have on driving would be a valuable asset to DOE, other federal agencies, and the trucking industry as they evaluate technologies for their effects on energy efficiency, safety, emissions, fleet management, and so forth. Capturing data on the nature and characteristics of heavy truck driving will lead to a better understanding of heavy truck operations and more representative duty cycles, factors which are critical for accurate analytical evaluations of new technologies.

Technology

An unprecedented suite of sensors and instruments is being used to measure and record over 90 different parameters (e.g., vehicle speed, acceleration, load, grade, wind velocity) from the operation of a heavy line-haul truck running on a dedicated route between Portland, Oregon, and Chicago, Illinois. The data collected will be analyzed to provide a basis for defining a heavy vehicle duty cycle.

This duty cycle represents the environment, speed, load, etc., experienced by heavy trucks and can serve as a universal basis for evaluating and comparing numerous figures of merit such as fuel economy, emissions, and performance. The project is led by Oak Ridge National Laboratory, with partners Dana Corporation of Kalamazoo, Michigan; Michelin Tire of Greenville, South Carolina; and support from Argonne National Laboratory.

Status

Two pilot runs from Bangor, Maine, to Miami, Florida, have been completed. The purpose of these runs was to evaluate the data acquisition systems and on-board data collection suites for field-hardening purposes. The pilot runs generated preliminary duty cycle information as a proof of concept. Results from the pilot runs will be utilized in a 12-month fleet-based test utilizing up to 10 instrumented class 8 tractor-trailers engaged in normal long-haul vocational activities.

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Energy Storage

Development of Advanced Cathodes

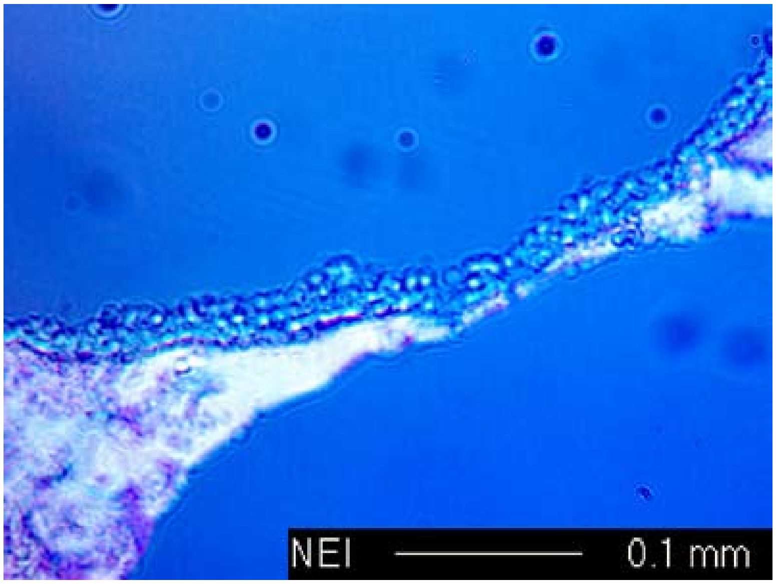

Figure 1. *Optical micrograph showing the cross-section of a LiFePO$_4$- coated graphite foam cathode. A graphite wall separates two large pores; the top surface of the wall is coated with a 30 µm–thick layer of LiFePO$_4$ particles.*

Background

Performance, affordability, and safety of batteries for electric vehicle and hybrid electric vehicle applications must continue to be improved for widespread use. The challenge to engineer battery materials that can withstand large fluctuations of composition, volume, and temperature over many, many cycles without loss of integrity and electrical continuity is formidable. A team of materials scientists at the Oak Ridge National Laboratory (ORNL) is focused on developing new composite electrode architectures and materials that may improve the thermal stability and cycleability of the battery cathode. For advanced lithium-ion batteries, cathodes composed of $LiFePO_4$ coated graphite foams are being evaluated. In addition, for the lithium-sulfur battery system, sulfur-copper composites have been studied.

Technology

Graphite foams pioneered at ORNL are expected to be superior current collectors for a variety of rechargeable battery chemistries due to their exceptional thermal and electrical conductivities, light weight, high surface area, and chemical stability. As the current collector for $LiFePO_4$ based cathodes, we estimate that a dense, thin coating of $LiFePO_4$ over the exposed and interior surfaces of a graphite foam sheet will give a capacity comparable to

Benefits

Advanced materials and designs for battery cathodes, formed as composites of the active and conductive materials, will improve cycle stability and thermal management of lithium batteries, without excessively compromising the high energy densities needed for vehicle applications.

that of conventional battery cathodes, yet the foam will provide superior thermal and electronic transport throughout the electrode.

To date, promising cycling has been achieved for $LiFePO_4$ slurry coated carbon foam prepared by a vendor, although the coatings are not uniform or as thin as needed. Advanced formulations and coating techniques are being developed at ORNL. With the graphite foams, the $LiFePO_4$ coating can be strongly bonded to the current collector via conventional heating or possibly by microwave processes, rather than simply pressed onto a metal foil as for conventional battery fabrication.

The theoretical energy density for lithium-sulfur batteries far exceeds that currently achievable in the lithium-ion systems. Because sulfur has a high electronic resistivity, it is essential to add a fine dispersion of a conductive additive, typically carbon black. Work to date shows that replacing the carbon additive with copper or copper sulfide will give a sulfur electrode with comparable theoretical energy density, but with potentially superior cycleability and higher utilization of the capacity. This is due to the high electronic conductivity and electrochemical activity of the Cu_2S and CuS phases. Copper sulfides have been prepared by electrochemical sulfidization of copper foils, films, and fibers. Composites of elemental sulfur and copper sulfides show good cycling for one or two cycles, but then deteriorate due to solubility of lithium sulfides in the electrolyte solution. The key challenges for future work require suppression of this dissolution and development of more robust composite architectures able to accommodate the volume changes during cycling.

Status

Future efforts will include development of new synthesis routes for superior $LiFePO_4$ coatings of the carbon foam. Using graphite foam, we hope to demonstrate effective thermal management for Li-ion batteries, without compromising the energy and power densities. Further improvement may be achieved by tailoring the density, cell size, and pore size for the foam morphology to maximize performance.

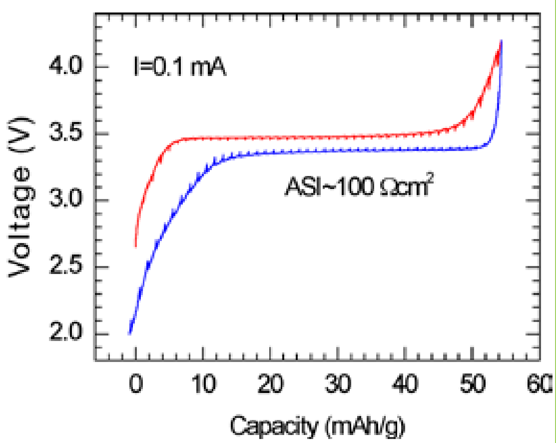

Figure 2. Charge/discharge cycle of a $LiFePO_4$-coated graphite foam cathode vs a lithium anode. Periodic relaxation of the battery during the cycle shows a low area-specific impedance.

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